Photonic bandgap fibers : scaling properties and biochemical sensing applications

Sun, Jian

2008

Sun, J. (2008). Photonic bandgap fibers : scaling properties and biochemical sensing applications. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/20671>

<https://doi.org/10.32657/10356/20671>

**NANYANG
TECHNOLOGICAL
UNIVERSITY**

**PHOTONIC BANDGAP FIBERS: SCALING PROPERTIES
AND BIOCHEMICAL SENSING APPLICATIONS**

SUN JIAN

SCHOOL OF CHEMICAL AND BIOMEDICAL ENGINEERING

2008

PHOTONIC BANDGAP FIBERS: SCALING PROPERTIES AND BIOCHEMICAL SENSING APPLICATIONS

SUN JIAN

SCHOOL OF CHEMICAL AND BIOMEDICAL ENGINEERING

A thesis submitted to the Nanyang Technological University
in partial fulfillment of the requirement for the degree of
Doctor of Philosophy

2008

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research done by me and has not been submitted for a higher degree to any other University or Institute.

.....
Date

.....
SUN JIAN

Acknowledgments

Although this thesis has a single author, this work would not have been possible without the help of many people. I have been fortunate enough to have several professors, colleagues and friends support me along the way. Without them, I am sure it would have been a far more difficult and tedious time for my graduate study.

It is impossible to mention all of the people whom I would like to thank. But first I want to express my sincere gratitude towards my advisor, Prof. Chan Chi Chiu, for making my study stimulating and enjoyable. By giving me a great deal of freedom to explore this research topic, he has also taught me how to effectively present and promote my own work. These skills will surely go a long way wherever my career takes me.

My thanks also go to Prof. Shum Ping, director of Network Technology Research Centre (NTRC). He and his research group have been instrumental in providing the equipment and assistance for many of my experiments. I am especially grateful for his providing me the chance to study in friendly and entertaining research centre.

I also thank the past and present members of NTRC. In particular, I owe special thanks to Dr. Yan Min, Dr. Yu Xia, Dr. Ren Guobin, Dr. Zhu Yinian and Dr. Alagappan A/L Gandhi. Their insight and wealth of knowledge and stimulating discussions gave a lot of inspiration to my research work. My sincere thanks also go to the rest of NTRC members. Because of them, my graduate study has always been exciting, enjoyable and unforgettable. I would also like to thank the technical staff in Network Technology Research Centre for their kind support and help in the past three years.

Special thanks go to our research group members, Ms. Ni Na and Ms. Zhang Yifan for their help and fruitful discussions. I have also made other great friends during my time at Nanyang Technological University. All of them have made life in Singapore more fun and memorable.

Finally, I am deeply grateful to my parents for their love, care and sacrifice for my education. Their understanding, encouragement and never ending support always stimulate me to further efforts. I would also like to thank my younger sister, Sun Xin, she was always proud of my every little success.

Sun Jian

January 2008

Table of Contents

Acknowledgmentsiii

Table of Contents v

Summary.....ix

List of Abbreviationsxi

List of Figures.....xiii

List of Tablesxix

Chapter 1 Introduction 1

 1.1 Motivation 1

 1.2 Objectives 3

 1.3 Originality of the investigation..... 4

 1.4 Layout of the Thesis 5

Chapter 2 Research Background7

 2.1 Introduction 7

 2.2 Optical techniques used in biochemical sensors..... 11

 2.2.1 Absorbance Measurements..... 12

 2.2.2 Fluorescence Measurement 13

 2.2.3 Refractometry 15

 2.2.4 Interferometry..... 18

 2.2.5 Surface Plasmon Resonance 20

 2.2.6 Photonic Crystals..... 21

 2.2.7 Liquid Crystals 23

2.3	Fiber-optic biochemical sensors	25
2.3.1	Introduction of Optical Fiber	25
2.3.2	Biochemical sensing applications.....	28
2.3.3	Advantages and Disadvantages	33
2.4	Photonic Crystal Fibers	34
2.4.1	Wave-guiding Mechanisms	34
2.4.2	Potential advantages	41
2.5	Numerical Analysis of Photonic Bandgap Fibers.....	43
2.5.1	Introduction	43
2.5.2	Fundamentals.....	44
2.5.3	Numerical Techniques	48
2.6	Chapter Summary	62
Chapter 3	Isotropic Photonic Bandgap Fibers.....	64
3.1	Introduction	64
3.2	Solid-core photonic bandgap fibers.....	65
3.2.1	Antiresonant reflecting optical waveguide model	65
3.2.2	Numerical analysis and verification	68
3.3	Hollow-core photonic bandgap fibers	71
3.3.1	Refractive index scaling law.....	71
3.3.2	Numerical Analysis and Verification	74
3.3.3	Vectorial effects on the bandgap formations.....	78
3.4	Chapter Summary	85
Chapter 4	Anisotropic Photonic Bandgap Fibers.....	87
4.1	Introduction	87

4.2	Refractive index scaling law for anisotropic PBGFs	89
4.2.1	All silica solid-core PBGF with NLC inclusions	94
4.2.2	High-index hollow-core PCF with NLC inclusions	95
4.3	Effect of liquid crystal alignment on bandgap formation.....	102
4.4	Solid-core anisotropic PBGFs	108
4.4.1	Photonic Bandgap Guiding ($n_b < n_e$ and $n_b < n_o$)	108
4.4.2	Hybrid guiding ($n_o < n_b < n_e$).....	116
4.5	Hollow core anisotropic PBGFs ($n_b > n_e$ and $n_b > n_o$)	125
4.6	Chapter Summary	130
Chapter 5	Photonic Bandgap Fibers based Biochemical Sensors.....	131
5.1	Introduction	131
5.2	Solid-core PBGFs for measuring high refractive index	132
5.2.1	Introduction	132
5.2.2	Experimental investigation of the performance.....	133
5.3	Hollow-core PBGFs for measuring of low refractive index	138
5.3.1	Experimental investigation of the performance.....	139
5.3.2	Discussion.....	145
5.4	Evanescent Wave Sensing	150
5.4.1	Theory and Simulation results.....	151
5.4.2	Experimental investigation of the performance.....	156
5.5	Discussion.....	160
5.5.1	Effect of temperature variation.....	160
5.5.2	Reusage of PBGFs.....	162
5.5.3	Background humidity, contamination and pollution	163

5.5.4 Other biochemical sensing applications 163

5.6 Chapter Summary 163

Chapter 6 Conclusions and Future Work 165

6.1 Summary of the investigation..... 165

6.2 Experimental Challenges 167

6.3 Suggestion of Future Work..... 168

6.3.1 Theoretical Work..... 169

6.3.2 Experimental Work..... 170

Author’s Publications 172

Bibliography 175

Summary

Photonic crystal fiber (PCF) is a new class of optical fiber based on the properties of photonic crystals [1]. One specific category of PCF is photonic bandgap fiber (PBGF), which confine light by bandgap effects. Recently, the perspectives for the design of tunable PBGF-based devices, such as tunable filters or dispersion compensators, are further widened, due to the introduction of isotropic (refractive index oil) and anisotropic materials (liquid crystal) into the holey regions of the fibers. These novel tunable properties are also promising for the sensing applications. In this thesis, the bandgap formation and tunability after the PBGFs are filled with isotropic and anisotropic materials are studied. In addition, experiments are carried out to verify the theoretical models and analyze the performance of PBGFs based biochemical sensors.

This thesis starts with a comprehensive review on the existing optical techniques used in biochemical sensors and their advantages and disadvantages. More specifically, the fundamental theory and biochemical sensing applications of conventional optical fibers are reviewed. PBGFs are proposed to tackle the disadvantages of conventional optical fibers, such as removing the cladding to enhance the performance. The classification and guiding mechanism of PBGFs are reviewed. Their potential advantages as biochemical sensors are also discussed. In addition, the fundamental equations and several numerical techniques are analyzed for solving the Maxwell's equations with different boundary conditions. The advantages and disadvantages concerning different numerical methods for the analysis of PCFs are also overviewed.

The theoretical models are developed for isotropic PBGFs. Based on the core and cladding compositions, the isotropic PBGFs are further divided into two categories, including solid-core PBGFs and hollow-core PBGFs. For solid-core PBGFs, the guiding mechanism can be understood by considering the antiresonant reflecting optical waveguide (ARROW) model. For the hollow-core PBGFs, the variations of bandgaps in response to the changes of refractive index can be described according to the refractive index scaling law. The theoretical models are both validated by numerical results.

Furthermore, the bandgap formation and variation of anisotropic PBGFs are studied. Particularly, the alignment of anisotropic material is an important issue which can alter the behavior of bandgaps. The investigation of anisotropic PBGFs mainly focuses on the nematic liquid crystal (NLC) infiltrated PBGFs. Three configurations of anisotropic PBGFs have been proposed and thoroughly studied.

At the final part of the thesis, experimental studies were carried out to realize the biochemical sensors by using PBGFs and verifying the theoretical models. The isotropic solid-core PBGFs are proposed for the measurement of high refractive index. The wavelength of transmission dip shifts 45nm in response to the refractive index change of 0.01 refractive index unit (RIU). The hollow-core PBGFs can be viewed as a complement to the solid-core PBGFs, which provide the measurement of refractive index ranging from 1.0 to 1.45 assuming the background material is silica. The wavelength of photonic bandgap edge (PBE) shifts 110nm with respect to the variation of refractive index of 0.02 RIU. In addition, with 95% light residing in the sample, the hollow-core PBGFs are good candidates for evanescent wave sensing.

List of Abbreviations

ARROW	Antiresonant reflecting optical waveguide
BPM	Beam Propagation Method
BBM	Biorthonormal Basis Method
CCA	Colloidal Crystal Arrays
EIM	Effective Index Method
FEM	Finite Element Method
FDM	Finite Difference Method
HF	Holey Fiber
IO	Integrated Optical
LC	Liquid Crystal
LFM	Localized Functions Method
MOF	Microstructured Optical Fiber
MPM	Multipole Method
NLC	Nematic Liquid Crystal
PBE	Photonic Bandgap Edge
PBG	Photonic Bandgap
PBGF	Photonic Bandgap Fiber
PC	Photonic Crystal
PCF	Photonic Crystal Fiber
PMMA	Polymethyl Methacrylate
PWM	Plane Wave Method

RIU	Refractive Index Unit
SC	Supercontinuum
SMF	Single Mode Fiber
SPR	Surface Plasmon Resonance
TIR	Total Internal Reflection

List of Figures

Fig. 2.1: Selection of scanning electron micrographs of PCF structures. (a) Details of the first working PCF which has a solid core surrounded by a triangular lattice of air holes. (b) First hollow-core PCF (c) First Bragg fiber. (d) Details of the Bragg fiber. The hollow core appears black, the PES layers and cladding grey, and the As₂Se₃ layers white [14]. 10

Fig. 2.2: A linear absorbing process [2] 13

Fig. 2.3: Excitation of a fluorophore at three different wavelengths (**EX 1, EX 2, EX 3**) does not change the emission profile but does produce variations in fluorescence emission intensity (**EM 1, EM 2, EM 3**) that correspond to the amplitude of the excitation spectrum [59]. 14

Fig. 2.4: Schematic diagram of a LPG [60]..... 15

Fig. 2.5: Transmission spectrum of a LPG written in SMF-28 fiber with $\Lambda=320\mu\text{m}$. The bands at 1496.6 nm (A), 1329.3 nm (B), 1243.8 nm (C) and 1192.1 nm (D) were used for refractive index experiments [62]. 16

Fig. 2.6: Experimental shifts in the four resonance bands of the LPG as a function of the index of the ambient medium [62]. 16

Fig. 2.7: Schematics of a Mach–Zehnder interferometer biosensor [2] 19

Fig. 2.8: (a) Kretschmann (ATR) geometry used to excite surface plasmons [10]; (b) Surface plasmon resonance curves. The left-hand-side curve is for just the silver film (labeled Ag); the right-hand-side curve shows the curve (labeled Ag/p-4-BCMU) shifted on the deposition of a monolayer Langmuir–Blodgett film of poly-4-BCMU on the silver film [2]. 21

Fig. 2.9: Inset, upper right: a CCA where the colloidal particles occur in a cubic array embedded within an acrylamide hydrogel. The pH dependence of the hydrolyzed CCA diffraction wavelength (see the inset on the upper left) is shown by the triangles. The solid line was calculated from the affine model and the broken line from the phantom model [66]. 23

Fig. 2.10: (a) A well-aligned liquid-crystal optical biosensor (b) undergoes a change in optical appearance after an enzymatic process removes the aligning lipid material. (c) Optical microscopy images show the changes in the optical texture of such a biosensor undergoing an enzymatic reaction; dark regions represent homeotropic alignment, and bright regions represent a tilted or planar alignment. Each of the wells is $\sim 283\text{ }\mu\text{m}$ wide with a depth of $\sim 20\text{ }\mu\text{m}$. [67]. 25

Fig. 2.11: Schematic diagram of a typical step-index fiber, n_{co} and n_{cl} are the refractive indices of the core and cladding, respectively.	26
Fig. 2.12: Schematic diagram of three types of optical fibers [69].	26
Fig. 2.13: Principle of total internal reflection [69].	28
Fig. 2.14: Evanescent wave biochemical sensor using partially clad fiber [3]. d_p is penetration depth.	29
Fig. 2.15: The fraction of modal power residing in the core for each of the first twelve modes as a function of V . The dashed curve is for the fundamental modes when $n_{co}=n_{cl}$ and V is fixed [70].	30
Fig. 2.16 Schematic of untapered and tapered fiber. A) Fiber probe with cladding stripped away from core. B) Step-tapered core to create V-number match between sensing and cladged regions. C) Continuously tapered core to maximize excitation light at surface. D) Combination tapered core to reach a V-number match quickly and subsequently maintain maximum excitation light at the fiber surface [3].	32
Fig. 2.17: Refractive indices of the core and cladding in (a) a step-index profile fiber and (b) index-guiding PCFs.	36
Fig. 2.18: Intensity distribution in the cladding of PCF for (a) short wavelength and (b) long wavelength [82].	37
Fig. 2.19: Schematic gap map of a photonic crystal cladding. Black-shaded areas are bandgap guiding regions.	38
Fig. 2.20: For wavelength in bandgap (a): A wave incident on a bandgap material [1] partially reflects off each layers of the structure [2]. The reflected waves are in phase and reinforce one another. They combine with the incident wave to produce a standing wave [3] that does not travel through the material. For wavelength not in bandgap (b): At wavelength outside the bandgap [1], the reflected waves are out of phase and cancel out each other [2], the light propagates through the material with only slightly attenuated [3].	39
Fig. 2.21: Transmission spectrum of a typical hollow-core PBGF [20].	40
Fig. 2.22: (a) The real-space (b) The reciprocal space of a 2D periodic structure with a hexagonal symmetry. R_1 and R_2 are the primitive lattice vectors, Λ is the lattice size, G_1 and G_2 are the reciprocal lattice vectors, the grey-area is the first Brillouin zone, Γ , M and K are the symmetry points [82].	52
Fig. 2.23: A general z-invariant waveguide.	55
Fig. 2.24: The 1D finite difference mesh [97, 99].	58

Fig. 2.25: An example of detail meshes which discretize the cross-section of a PCF [87].	61
Fig. 3.1: Solid-core PBGF with its air holes arranged in a triangular lattice. Black regions represent high-index inclusions, where $n_a > n_b$	65
Fig. 3.2: Plot of Bessel function of the first kind, $J_\alpha(x)$, for integer orders $\alpha=0, 1, 2, 3...$	68
Fig. 3.3: Enlarged gap map with normalized wavelength ranging from 0.125 to 0.3. Inset figure: Full gap map of the photonic crystal cladding.....	69
Fig. 3.4: Hollow-core PBGF with its air holes arranged in a triangular lattice. Black regions represent air.....	72
Fig. 3.5: Transmission spectrum for a PBG fiber filled with water. Inset figure: Shaded regions are gap regions [127].	75
Fig. 3.6: (a) Transmission spectra for different index profiles within the circular holes. (b) Wavelength shifts of two edges of the transmission window [127]......	76
Fig. 3.7: Variations of the bandgaps with different air-filling fractions as the refractive index changes [127]......	78
Fig. 3.8: Photonic band structures of (a) scalar wave approximation, (b) semi-vector approximation and (c) full-vector case. ($f=0.7, n_a=1, n_b=1.45, \beta=10$) [127]......	81
Fig. 3.9: Positions of PBGs on the low-index line vs. refractive index contrast. Shaded regions: full-vector PWM. Dashed lines: scalar PWM. ($n_b=1.45, n_a=1.45-\Delta n$) [127].	82
Fig. 3.10: Locations of primary PBGs on the low-index line vs. refractive index contrast for different air-filling fractions. Shaded regions: full-vector PWM. Dashed lines: scalar PWM. ($n_b=1.45, n_a=1.45-\Delta n$) [127]......	84
Fig. 4.1: (a) All silica solid-core PBGF with NLC inclusions, (b) high-index hollow-core PBGF with NLC inclusions.....	90
Fig. 4.2: Gap map of the PC cladding in with $\epsilon_a=\text{diag}(n_o^2, n_o^2, n_e^2)$. Arrows indicate the modal cutoffs of an individual cylindrical rod with $\epsilon_a=\text{diag}(n_o^2, n_o^2, n_e^2)$	95
Fig. 4.3: Gap maps of the PC claddings with $\epsilon_a=\text{diag}(n_o^2, n_o^2, n_e^2)$ and $\epsilon_a=n_o^2$	96
Fig. 4.4: Ideal anisotropic PBGF derived from Fig. 4.1(b).	98
Fig. 4.5: PBG-guiding wavelength ranges as a function of n_e	99
Fig. 4.6: PBG-guiding wavelength ranges as a function of $\sqrt{n_b^2 - n_o^2}$	101

- Fig. 4.7: (a) Cross section of the anisotropic PBGF. (b) NLC with optic axis along z direction. (c) NLC with optic axis along y direction. 102
- Fig. 4.8: (a) Gap map of the PC cladding with $\epsilon_a = \text{diag}(n_o^2, n_e^2, n_o^2)$ by using full-vectorial model and (b) by using the approximation which ignores the coupling effect. Arrows indicate the modal cutoffs of an individual cylindrical rod with $\epsilon_a = n_o^2$ and $\epsilon_a = \text{diag}(n_e^2, n_e^2, n_o^2)$, respectively. 106
- Fig. 4.9: Modal dispersion curves of fundamental modes as a function of the wavelength. Inset figures: field distributions of E_x and E_y 107
- Fig. 4.10: Transmission spectra for an isotropic PBGF and an anisotropic PBGF. The analytical cutoff wavelengths are marked as vertical arrows. 110
- Fig. 4.11: Modal intensity distribution and electric vector distribution for (a) isotropic PBGF at $0.787\mu\text{m}$, anisotropic PBGF (b) at $0.787\mu\text{m}$ and (c) $0.886\mu\text{m}$ 111
- Fig. 4.12: Transmission spectra for the solid-core anisotropic PBGF with different pitches. 112
- Fig. 4.13: Transmission spectra for the solid-core anisotropic PBGF with different number of rings. 114
- Fig. 4.14: Exact solution of the cutoff wavelengths vs. κ_{co} 115
- Fig. 4.15: Comparison of exact solution and cosine approximation of modal cutoffs... 116
- Fig. 4.16: Gap map of the PC cladding with optic axis of NLC inclusions along y direction. Inset figure: IBZ. 118
- Fig. 4.17: Gap maps of E_x and E_y which correspond to the band structure of the PCs with $\epsilon_a = \text{diag}(n_o^2, n_o^2, n_o^2)$ and $\epsilon_a = \text{diag}(n_e^2, n_e^2, n_o^2)$, respectively. 119
- Fig. 4.18: Dispersion curves of guided modes as a function of the wavelength for x and y polarizations. 120
- Fig. 4.19: Transmission spectra for x and y polarizations. 121
- Fig. 4.20: Mode intensity of x -polarized fundamental modes at the wavelength of (a) 780nm , (b) 988nm and (c) 1550nm and of y -polarized fundamental modes at the wavelength of (d) 780nm , (e) 988nm and (f) 1550nm 123
- Fig. 4.21: Modal birefringence as a function of the wavelength. Shaded region represents the wavelength range outside the bandgaps of E_y . Inset, difference of the confinement losses of E_x and E_y within the wavelength range of $0.8\mu\text{m}$ to $1.2\mu\text{m}$ 125

Fig. 4.22: (a) Gap map of the PC containing NLC with optic axis aligned along y direction. Inset figure: IBZ. (b) Approximated gap maps of E_x and E_y which correspond to the band structure of the PC claddings with $\epsilon_a=n_o^2$ and $\epsilon_a=n_e^2$, respectively.	129
Fig. 5.1: Schematic diagram of the experiment setup. (SC light source: Supercontinuum light source; OSA: optical spectrum analyzer; PBGF: photonic bandgap fiber). ..	134
Fig. 5.2: Transmission spectrum of the solid-core PBGF with ambient refractive index of 1.52.	135
Fig. 5.3: Transmission spectrum of the solid-core PBGF with ambient refractive index of 1.64.	136
Fig. 5.4: Wavelength shifts of transmission dips. Lines represent the analytical results.	137
Fig. 5.5: Schematic diagram of the experiment setup. (SC light source: Supercontinuum light source; OSA: optical spectrum analyzer; PBGF: photonic bandgap fiber). ..	139
Fig. 5.6: Transmission spectra of (a) 20cm and (b) 50cm hollow-core PBGFs without filling.	141
Fig. 5.7: Normalized transmission spectra taken (a) before and (b) after filling with water.	142
Fig. 5.8: (a) Normalized transmission spectra of the hollow-core PBGF with three different ambient refractive indices ranging from $n_a=1.35$ to $n_a=1.39$. (b) Wavelength shift of the falling PBE plotted as a function of ambient refractive index n_a	143
Fig. 5.9: Simplified model of a hole in the cladding after the formation of a biolayer. ..	146
Fig. 5.10: Wavelength shift of the falling PBE as a function of biolayer thickness.....	147
Fig. 5.11: Wavelength shift of the falling PBE as a function of the biolayer refractive index	148
Fig. 5.12: Hollow-core PBGF with air holes arranged in a triangular lattice. Black regions represent air.	152
Fig. 5.13: Electric field distributions (a) at $\lambda_0=1.55\mu\text{m}$ before filling of pure water and (b) $\lambda=0.853\mu\text{m}$ after the filling of pure water.....	155
Fig. 5.14: Transmission spectra of two hollow-core PBGFs with a $0.2\mu\text{M}$ Alexa Fluor 700 labeled DNA solution (solid curve) and pure water for reference (dotted curve), respectively. Inset, derived absorbance in the sample containing the Alexa Fluor 700 labeled DNA Oligo solution.	158

Fig. 5.15: Absorption measurement for different concentrations of Alexa Fluor 700 labeled DNA solutions. 160

List of Tables

Table 2-1: Overview of advantages and disadvantages concerning different numerical methods for the analysis of PCFs [108]. 49

Table 4-1: Modal cutoffs of a step-profile uniaxial fiber with an anisotropic core and an isotropic cladding. 94

Table 4-2: Modal cutoffs of a step-profile uniaxial fiber with an isotropic core and an anisotropic cladding..... 97

Chapter 1

Introduction

1.1 Motivation

Since the birth of the field of optical biochemical sensors, the pace of evolution in this field has been swift [2]. Optical biochemical sensors utilize optical techniques to detect and identify chemical or biological species. They offer a number of advantages over conventional sensing methods [2, 3]. For example, they offer the advantage of real-time monitoring and remote sensing with no electrical interference. Additionally, they offer multiple channels or multiparameters detection with compact sensor design. The minimally invasive for in vivo measurements is another advantage that they can provide.

The invention of optical fibers boosted the development of optical chemical sensors [4-6]. The subject has been under extensive investigation over more than two decades. Fiber-optic biochemical sensors are the most widely studied optical biochemical sensors [2]. There are several reasons for the popularity of fiber-optic biochemical sensors. Perhaps the most significant is that they can provide long interaction length and adaptability for optical instruments, especially in spectrometry. This is becoming very important in the development of remote and continuous sensing in gases or liquid without sampling [7-9]. Besides, optical fibers can act as a platform for the development of

various optical techniques, such as absorption spectroscopy, Raman spectroscopy and Surface Plasmon Resonance [4-6, 10]. The flexibility in the selection of optical techniques makes it easy to change the configuration of fiber-optic biochemical sensing system to suit for the user's specifications. The wavelength multiplex capacity of the optical fiber also enables multiple analytes determinations in a single central unit.

A large variety of fiber-optic biochemical sensors detect and identify chemical or biological species based on the interaction of the evanescent wave with the sensing layer deposited on the surface of the optical fibers [2, 4, 5]. Evanescent wave is the electromagnetic field that extends away from the surface of the light guiding medium, i.e. optical fibers. The evanescent wave absorption is inversely proportional to the diameter of the optical fibers [11]. As the intensity of evanescent waves decays exponentially with the distance from the interface at which the evanescent waves are formed, part of the cladding of optical fiber is removed in order to achieve a strong penetration of evanescent waves into the analytes [3, 11]. This makes the fiber to be easily broken. In addition, for fluorescence spectroscopy, the thin cladding of the optical fibers greatly deteriorates the efficiency of coupling of fluorescence emission from the surface into the optical fibers. These limitations are related to the nature of conventional optical fibers.

Since the demonstration of first experimental demonstration of photonic crystal fiber (PCFs) in 1996 by Knight *et al.* [12], the optical properties and the fabrication of such fibers have attracted significant attentions [13, 14]. The fiber structure with a lattice of air holes running along the length of fiber provides a large variety of novel optical properties

and improvements compared to the standard optical fibers. Photonic bandgap fibers (PBGFs) are members of PCFs, which guides light by the photonic bandgap (PBG) effect. At least two characteristics of PBGFs enable their applications in biochemical sensing areas. Firstly, in a PBGF, light can be guided in a low-index core filled with air or analyte samples. Thus, more than 90% optical power could propagate through the analyte and it is not required to remove the cladding of the PBGF. This greatly improves the performance of the conventional fiber-optic biochemical sensors in terms of not only efficiency but also robustness. Secondly, the transmission spectra of PBGFs are characterized by having several transmission windows. The locations of these transmission windows show strong dependence on the refractive index contrast. This offers the possibility of designing label-free biochemical sensors through refractive index measurement.

1.2 Objectives

The objectives of the thesis are to investigate the variations of refractive index on the modifications of bandgaps of both isotropic and anisotropic PBGFs. This is because that the measurement of refractive index is a label free detection technique which allows monitoring the interactions of various biomolecule complexes without using fluorescence labels or radio labels. An important issue is to find explicit expressions, which could describe the scaling of bandgaps when the refractive index changes. Besides refractive index scaling, another issue facing anisotropic PBGFs is the alignment of anisotropic

material, which is also worth to be investigated and applied in the future biochemical sensor design. These systematic modeling and theoretical analysis provide a theoretical guidance for the biochemical design and analysis. Experimental demonstration of the potential biochemical sensing application is also crucial for verifying the theoretical model and providing prototypes for the design of future PBGFs based biochemical sensors.

1.3 Originality of the investigation

The main original works in this thesis may be summarized as follows:

1. Theoretical investigation and demonstration of the bandgap formation of isotropic PBGFs, including solid-core and hollow-core PBGFs.
2. Theoretical investigation of the effect of liquid crystal alignment on the formation of anisotropic PBGFs.
3. Theoretical investigation of the refractive index scaling properties of anisotropic PBGFs.
4. Theoretical investigation of the bandgap formation for different configurations of anisotropic PBGFs.
5. Experimental investigation and demonstration on the detection of high refractive index, by using solid-core PBGFs, which relies on the measurement of the wavelength shifts of the transmission dips in the transmission spectrum.

6. Experimental demonstration of the possibility of using hollow-core PBGFs as a label-free biochemical sensor by detecting the wavelength shifts of the PBGs. A simplified three-layer model of a hole in the cladding is proposed in order to simulate the biolayer effect. The sensitivity is estimated to be around 0.1nmol/L.
7. Experimental demonstration of the sensitivity enhancement by using hollow-core PBGFs as an evanescent wave sensor. The sensitivity can be evaluated by using refractive index scaling law.

1.4 Layout of the Thesis

This thesis is organized as follows:

1. Chapter 2 overviews the research background. After reviewing various optical techniques used in optical biochemical sensors, the most widely studied optical biochemical sensors, namely, fiber-optic biosensors are reviewed, including the pros and cons. Unique features of the PBGFs, which make them very attractive for biochemical sensing applications, are discussed.
2. Chapter 3 introduces the fundamental equations for optical waveguides and numerical techniques for analyzing photonic crystal fibers. An overview of the pros and cons of various numerical techniques is presented. The vector wave equations for plane wave methods, beam propagation method, finite difference method and finite element method are also described.

3. Chapter 4 describes the refractive index scaling property of isotropic solid-core and hollow-core PBGFs, which are the basic principles for designing biochemical sensors. The relationship between the locations of the photonic bandgaps and refractive index has been investigated theoretically.
4. Chapter 5 describes the refractive index scaling property anisotropic solid-core and hollow-core PBGFs. The alignment of liquid crystal on the bandgap formation has also been theoretical studies. These constitute the theoretical fundamentals for the design of novel anisotropic PBGFs based biochemical sensors. In particular, the bandgap formation of three types anisotropic PBGFs have been investigated.
5. Chapter 6 presents the experimental investigation on the performance of PBGFs based biochemical sensors. Three kinds of sensors have been demonstrated including the measurement of high refractive index, low refractive index and evanescent wave sensing.

Chapter 2

Research Background

2.1 Introduction

Biochemical sensors are analytical devices that can detect chemical or biological species or a microorganism [2, 3, 5, 15, 16]. In the wake of the terrorist attacks in recent years there is a sudden demand for effective diagnostic tools, namely biochemical sensors, for the rapid identification of biowarfare agents, not only for the military sector but for the civilian sector [6, 17-19]. In addition, the constant health danger posed by new strands of microbial organisms and spread of infectious diseases is another concern requiring biochemical sensing for detecting and identifying them rapidly. The biochemical sensor system can identify known, previously unknown, and bioengineered infectious agents for use in biowarfare defense; identify and track disease patterns for use in epidemiological surveillance; and aid in solving crimes involving infectious agents for use in microbial forensics. The biochemical sensor system also has the potential to be used in pharmaceutical process control, hospital-associated infection control and infectious disease diagnostics.

The ideal biochemical sensor for counter-terrorism and defense applications needs to have high sensitivity and wide applicability to different types of biowarfare agents, while

remaining compact, easy to use, fast, and reliable (no false positives). Optical biochemical sensors utilize optical techniques to detect and identify chemical or biological species. They offer a number of advantages such as the ability for principally remote sensing with high selectivity and specificity and the ability to use unique biorecognition schemes. More in particular, progress of fiber optics has made fiber-optic biochemical sensors to be one of the most widely studied optical biochemical sensors during the past two decades [2]. The advantages of the fiber-optic biochemical sensors are easily to be identified, such as long interaction length, compactness (small sample volume), large overlap between the light and sample, and compatibilities with catheters or endoscopes for in vivo biochemical sensing.

Photonic crystal fibers (PCFs) have attracted significant attentions recently because of their unique properties [13, 14]. To date, PCFs have evolved into many types, which are characterized for different applications [13, 20]. Although PCFs deviate much in structures, such fibers are characterized by having a pattern of microstructure from two or more materials (usually air and silica) along the entire length of the fiber. They have been demonstrated to perform better in applications such as high nonlinearity and high birefringence. In addition, some hollow-core PCFs have thrived in areas like high power pulse delivery and atom guiding. The holey structure of PCFs is also expected to perform better in the biochemical sensing applications than the conventional optical fibers.

The term "photonic crystal fiber" was coined by Philip Russell [13]. However, other terms such as microstructured optical fiber (MOF) are also used and the nomenclature in

the field is not entirely consistent [21]. These include holey fiber (HF), hole-assisted fiber, photonic-bandgap fiber (PBGF) and Bragg fiber. HF is used to address the PCFs using air holes in their cross-sections. Hole-assisted fiber represents the PCFs guiding light by a conventional high-index core modified by the presence of air holes. PBGF is addressed for all PCFs that confine light by bandgap effects and Bragg fiber represents the PBGF formed by concentric rings of multilayer film. Although the names deviate much, they are defined from either structure point of view or optical-property point of view. For example, PCF, MOF and HF are defined from structure point view. PBGF and Bragg fiber are defined from optical-property point of view.

Generally speaking, such fibers are characterized by having a periodically arranged microstructure from two or more materials (usually air and silica) over much of the cross-section (normally uniform along the fiber length), usually as a "cladding" surrounding a core (or several cores). For example, the fibers first demonstrated by Russell consisted of a hexagonal lattice of air holes in a silica fiber, with a solid [12] or hollow core [20] at the center where light is guided. Other arrangements include concentric rings of two or more materials, first proposed as "Bragg fibers" by Yeh and Yariv [22], a variant of which was recently fabricated by Temelkuran et al [23]. The variation of the geometry can be viewed from Fig. 2.1.

Fig. 2.1: Selection of scanning electron micrographs of PCF structures. (a) Details of the first working PCF which has a solid core surrounded by a triangular lattice of air holes. (b) First hollow-core PCF (c) First Bragg fiber. (d) Details of the Bragg fiber. The hollow core appears black, the PES layers and cladding grey, and the As_2Se_3 layers white [14].

Generally, such fibers are constructed by the same general principles as other optical fibers. The first step is to construct a "preform" on the scale of centimeters in size, and then heats the preform and draws it down to a much smaller diameter, shrinking the preform cross-section but maintaining the same features. In this way, kilometers of fiber can be produced from a single preform. Excepting silica, other glasses have also been used to obtain particular optical properties [24-26]. There is also a growing interest in making them from polymer, which makes it easy to fabricate a wide variety of structures, including graded index structures, ring structured fibers and hollow core fibers. In addition, compound glasses, such as sulphides, halides and heavy metal oxide glasses, have been used to extend wavelength transmission range [27].

In this chapter, the optical techniques used in biochemical sensors are described in Section 2.2. The basic properties of the fiber-optic biochemical sensors are presented in Section 2.3. An introduction of PCFs and the potential advantages for biochemical sensing applications are presented in Section 2.4. Numerical Analysis of Photonic Bandgap Fibers is described in Section 2.5. A chapter summary is given in Section 2.6 .

2.2 Optical techniques used in biochemical sensors

An optical biochemical sensor senses the presence of an analyte and creates an optical signal by the optical transducer [15, 28]. Optical transduction utilizes changes in optical properties such as phase, amplitude, and frequency because of the selective binding of an analyte with the biorecognition element. The variety of the transduction mechanisms enables the design of various types of optical biochemical sensors, some of which are already in practice. Generally, the optical techniques used in biochemical sensors can be classified as absorbance measurements [29], fluorescence measurements [30, 31], refractometry [4, 32, 33], interferometry [34-37], surface plasmon resonance [6, 10, 38-41], photonic crystals [42-46] and liquid crystals [47-50].

Several types of label-free fiber-optic biosensors have been investigated over the past few years. For example, surface plasmon resonance (SPR) sensors allow the detection of selective binding by measuring the change of the refractive index near the surface of a gold film [51]. However, this method required the use of a special metal layer (gold or silver) on which the bioactive agent cannot be easily and firmly bound [52]. Long period

grating (LPG) based biosensors have been demonstrated by immobilizing antibodies on the surface of the fiber and monitoring the change in refractive index during the antigen-antibody reaction [53, 54]. More recently, two-dimensional photonic crystals (PCs) were of particular interest for biochemical sensing applications, which were based on the measurement of the shift of the resonance wavelength under the influence of the variation of refractive index [55-58]. Since most of the label-free approaches rely on refractive index measurement, a highly sensitive fiber-optic biosensor is one kind of sensor that is very sensitive to the change in the refractive index.

2.2.1 Absorbance Measurements

For absorption, a broad band light source generally is used, and its transmission (and hence, attenuation or absorption) is obtained as a function of frequency or wavelength. The change in light intensity due to absorption is determined by the number of absorbing species in the optical path and is related to the concentration of the absorbing species via the Beer-Lambert relationship, according to which the attenuation of an incident beam of intensity I_o at wavelength λ is described by an exponential decay whereby the output intensity I is given as [2]

$$I(\lambda) = I_o(\lambda)e^{-\varepsilon(\lambda)bc} \quad (2.1)$$

The more frequently used coefficient $\varepsilon(\lambda)$ expressed in $L \text{ (liters)} \text{ mol}^{-1} \text{ cm}^{-1}$ is called the molar extinction coefficient at wavelength λ ; c is the molar concentration (mol/L).

Fig. 2.2: A linear absorbing process [2]

Absorption technique is a relatively simple biochemical sensing technique. However, the main limitations are the small dynamic range of the measuring instrument and interference from background absorptions.

2.2.2 Fluorescence Measurement

Fluorescence is one of the most successful optical techniques in biochemical sensors. It occurs when molecules are excited at a specific wavelength and re-emit radiation at a lower energy, i.e., a longer wavelength. This type of transduction is usually applied in enzymatic biochemical sensors in which the analyte is biocatalytically converted to a product, or reacts with a compound with optical properties, or that induces an optical signal.

There are four essential elements of fluorescence detection systems, including an excitation source, a fluorophore, wavelength filters to isolate emission photons from excitation photons and a detector that registers emission photons and produces a recordable output, usually as an electrical signal or a photographic image [59]. Fluorescence intensity is quantitatively dependent on the same parameters as absorbance, which are defined by the Beer–Lambert law as the product of the molar extinction

coefficient, optical path length and solute concentration [59]. With few exceptions, the fluorescence excitation spectrum of a single fluorophore species in dilute solution is identical to its absorption spectrum [59]. Under the same conditions, the fluorescence emission spectrum is independent of the excitation wavelength, due to the partial dissipation of excitation energy during the excited-state lifetime. The emission intensity is proportional to the amplitude of the fluorescence excitation spectrum at the excitation wavelength, which is shown in Fig. 2.3.

Fig. 2.3: Excitation of a fluorophore at three different wavelengths (EX 1, EX 2, EX 3) does not change the emission profile but does produce variations in fluorescence emission intensity (EM 1, EM 2, EM 3) that correspond to the amplitude of the excitation spectrum [59].

The light emitted by the sensing element containing the fluorescent indicator will be collected and then be filtered and delivered to the detector. Light intensity, decay time, polarization, or phase of the emitted radiation can be selected as the analytical property used to evaluate the concentration of the analyte. The fluorescence technique offers extremely high sensitivity, but it is difficult to be multiplexed and requires fluorescently-labeled biomolecules.

2.2.3 Refractometry

The measurement for the change of refractive index is of considerable interest in determining the variation of concentration of chemical or biochemical species in a simple mixture of test medium. This is because the change of concentration will affect the density and atomic interaction of the solution and thus will alter the refractive index. Refractometry is the method of measuring substances' refractive index in order to assess their composition or purity.

Fig. 2.4: Schematic diagram of a LPG [60]

There are a lot of optical techniques developed for measuring the refractive index. For example, long period fiber gratings (LPGs) consist of a periodic perturbation of the properties of the optical fiber, generally of the refractive index of the core, with a period typically in the range $100\ \mu\text{m}$ to $1\ \text{mm}$ [53, 60, 61]. The schematic diagram for a LPG is demonstrated in Fig. 2.4. The high attenuation of the cladding modes results in the transmission spectrum of the fibre containing a series of attenuation bands centered at discrete wavelengths, each attenuation band corresponding to the coupling to a different cladding mode. Examples of the transmission spectra of LPGs are shown in Fig. 2.5.

Fig. 2.5: Transmission spectrum of a LPG written in SMF-28 fiber with $\Lambda=320\mu\text{m}$. The bands at 1496.6 nm (A), 1329.3 nm (B), 1243.8 nm (C) and 1192.1 nm (D) were used for refractive index experiments [62].

Fig. 2.6: Experimental shifts in the four resonance bands of the LPG as a function of the index of the ambient medium [62].

The refractive index sensitivity of LPGs arises from the dependence of the phase matching condition upon the effective refractive index of the cladding modes. The effective indices of the cladding modes are dependent upon the difference between the

refractive index of the cladding and that of the medium surrounding the cladding. The central wavelengths of the attenuation bands thus show a dependence upon the refractive index of the medium surrounding the cladding, provided that the cladding has the higher refractive index. Fig. 2.6 shows the experimental shifts in the four resonance bands of the LPG as a function of the index of the ambient medium [62]. The detection of one specific molecule species from the others is possible. LPG based biosensors have been demonstrated by immobilizing antibodies on the surface of the fiber and monitoring the change in refractive index during the antigen-antibody reaction [53, 54].

Refractometry is a label free detection technique which allows monitoring the interactions of various biomolecule complexes without using fluorescence labels or radio labels. It thus improves the flexibility and allows measuring both static and dynamic binding interactions among the biomolecules.

However, there are several challenges which are thrown to the researchers working in this area, such as the method used to detect specific molecules from groups of molecules [4-6, 10, 63-65]. Bimolecular recognition molecules may exhibit affinity to similar types of other unwanted molecules present in a given system. These unwanted molecules will react with the biosensors and will alter the refractive index, hence, affecting the other different important parameters such as sensitivity, detection accuracy, reproducibility, etc., of the biosensor. If the concentration of unwanted molecule is high, then sensor response is more affected by it rather than by the molecule which we want to detect. The other challenge lies in the nonspecific interactions between the sensor surface

with the unwanted molecules and the background refractive index variations. These variations can be owing to the temperature, humidity, and compositional fluctuations. These important issues restrict the use of refractive index sensing in the laboratory environment. To use the biosensors in field, mobile analytical systems need to be developed, which should provide environmental control and enable rapid detection of given biological entity. Future developments of these systems require significant advances in miniaturization of biosensing platform, high specificity, robustness, and user friendliness.

2.2.4 Interferometry

An interferometric biochemical sensor utilizes interference between the light from a waveguiding channel with a sensing layer on its surface, and that from a reference channel. In this type of sensing, the binding of an analyte with a biorecognition element that is immobilized on the surface of the sensing waveguide channel induces the variations of ambient refractive index.

Fig. 2.7: Schematics of a Mach-Zehnder interferometer biosensor [2]

The most commonly used technique for biosensing has been that of a Mach-Zehnder interferometer. Fig. 2.7 shows the schematics of such a biosensor [2]. The sample arm exhibits specific binding with the biological analyte, based on the specificity of the immunoglobulin (IgG) that is immobilized on its surface. An optical beam I_{in} is split into two parts, which travel through two arms (channel waveguides or fibers)—that is, the reference arm and the sample arm of the interferometer. If the two arms are not exactly identical, the phase-shift introduced in the two arms are different. The sample arm forms the sensing area of the interferometer. Therefore, when the two beams from these two arms are recombined near the output port, the output intensity I_{out} is modulated due to interference between them. If the relative phase shift between the reference and the sample arms is $\Delta\Phi$, the output intensity is given as

$$I_{out} = I_{in} (1 + M \cos \Delta\Phi) \quad (2.2)$$

where M is the modulation factor and $\Delta\Phi$ is the relative phase shift between two arms. It can detect the refractive index changes within the penetration depth of the evanescent field. This technique has the merit of high sensitivity, but it requires a highly stable environment and it is not easily to be multiplexed.

2.2.5 Surface Plasmon Resonance

Surface plasmon resonance sensors are perhaps the most extensively utilized optical biochemical sensors. It can be viewed as an extension of the evanescent wave sensing, which can monitor the refractive index as well as the thickness of a surface layer.

In principle, the surface Plasmon resonance (SPR) technique is an extension of evanescent wave sensing, except that a planar waveguide is replaced by a metal–dielectric interface [2]. Surface plasmons are electromagnetic waves that propagate along the interface between a metal and a dielectric material such as organic films. Since the surface plasmons propagate in the frequency and wave-vector ranges for which no light propagation is allowed in either of the two media, no direct excitation of surface plasmons is possible. The most commonly used method to generate a surface Plasmon wave is attenuated total reflection (ATR).

The Kretschmann configuration of ATR is widely used to excite surface plasmons, which is shown in Fig. 2.8(a). This method relies on the measurement of the reflectance as a function of the incident angle of the light that is reflected from the metal-coated surface. At a critical angle, θ_r , a surface plasmon can be excited propagating along the

metal surface, which leaves a sharp minimum in the reflectance. The angle is a strong function of the dielectric profile of the immediate vicinity of the metal layer as shown in Fig. 2.8(b).

Fig. 2.8: (a) Kretschmann (ATR) geometry used to excite surface plasmons [10]; (b) Surface plasmon resonance curves. The left-hand-side curve is for just the silver film (labeled Ag); the right-hand-side curve shows the curve (labeled Ag/p-4-BCMU) shifted on the deposition of a monolayer Langmuir-Blodgett film of poly-4-BCMU on the silver film [2]

The performance of the SPR technique is dependent on the selected metal, the corresponding signal processing technique and the measured parameters, including the angle for the reflectivity minimum, the minimum value of reflectivity, and the width of the resonance curves. The SPR technique has several distinct advantages, such as no labeling required, real-time monitoring and small amount of materials required for typical analysis. However, the use of a special metal layer, such as gold or silver, increase the cost and makes the bioactive agent difficult to be bound on the metal surface.

2.2.6 Photonic Crystals

A photonic crystal is a periodic arrangement of macroscopic dielectric media. Analogous to the electronic materials, the lattice might introduce gaps into the energy band structure

of the crystal, so that photons are forbidden to propagate with certain energies in certain directions. In other words, a photonic crystal can reflect light of any polarization incident inside the bandgap, which is a certain frequency range. The reflected frequency range is strongly dependent on the dielectric difference as well as the lattice structure of the photonic crystal. Therefore, any variation in the lattice structure or the dielectric difference can produce a shift in the frequency range, which thus can be used for the biochemical sensing applications.

For example, Asher and co-workers fabricated a three-dimensional periodic structure of colloidal crystal arrays (CCA) of highly charged polystyrene spheres within a hydrogel [46, 66]. The CCA self-assembly results from electrostatic repulsion between monodisperse, highly charged colloidal particles, which forms a soft fluid material where the particles occur in a face-centered cubic or body-centered cubic array. These photonic crystal sensing materials have the potential utility to sense any analyte, provided recognition elements can be synthesized and attached to the hydrogel to couple analyte binding to hydrogel volume-phase transitions. Since hydrogel swells and shrinks reversibly in the presence of certain analytes such as metal ions or glucose. This leads to a change in the diffracted wavelength, which is shown in Fig. 2.9.

Fig. 2.9: Inset, upper right: a CCA where the colloidal particles occur in a cubic array embedded within an acrylamide hydrogel. The pH dependence of the hydrolyzed CCA diffraction wavelength (see the inset on the upper left) is shown by the triangles. The solid line was calculated from the affine model and the broken line from the phantom model [66].

2.2.7 Liquid Crystals

The anisotropic properties of liquid crystals (LCs) are explored to create an extremely sensitive technology for the real-time detection of nanometer-sized particles, including proteins and viruses [47-49, 67]. Such sensors consist of a thin film of a LC, confined between two aligning surfaces. They can report the presence of specific biological particles by detection of the orientation of LC using a polarizing microscope or the naked eye. This kind of sensor exploits two properties of the orientation of liquid crystals: the elasticity and the sensitivity to confining surfaces. When a sufficiently high percentage of the walls are covered by nanoparticles, such as proteins and viruses, the elasticity of the liquid crystal cannot overcome the highly inhomogeneous anchoring conditions imposed

by the nanoparticles. Hence, the LCs orient in order to relax the energy towards a uniform state.

For example, Fig. 2.10 depicts the detection of an enzymatic reaction whereby a biosensor containing an enzymeladen liquid-crystal layer detects enzymatic activity after the introduction of a lipid-containing aqueous solution. The liquidcrystal molecules possess a homeotropic alignment at the aqueous interface before any reaction occurs (Fig. 2.10a). As the reaction takes place, regions of the interface become depleted of lipids, inducing an orientational change in the liquid-crystal molecules to a planar alignment (Fig. 2.10b). During this transition, the optical appearance of the biosensor will change when viewed between crossed polarizers (Fig. 2.10c) [67].

The sensitivity of the sensor can be tuned by controlling the temperature, the dimensions of the film, and the pattern of the adsorption sites. These sensors are small (approximately 1 inch square), inexpensive, and will not require a great deal of medical knowledge or experience to interpret.

Fig. 2.10: (a) A well-aligned liquid-crystal optical biosensor (b) undergoes a change in optical appearance after an enzymatic process removes the aligning lipid material. (c) Optical microscopy images show the changes in the optical texture of such a biosensor undergoing an enzymatic reaction; dark regions represent homeotropic alignment, and bright regions represent a tilted or planar alignment. Each of the wells is $\sim 283\text{ }\mu\text{m}$ wide with a depth of $\sim 20\text{ }\mu\text{m}$. [67].

2.3 Fiber-optic biochemical sensors

2.3.1 Introduction of Optical Fiber

2.3.1.1 Definition and Classification

An optical fiber is a cylindrical dielectric waveguide that transmits light along its axis, by the process of total internal reflection [68]. The fiber consists of a core surrounded by a cladding layer. To confine the optical signal in the core, the refractive index of the core

must be greater than that of the cladding. The boundary between the core and cladding may either be abrupt, in step-index fiber, or gradual, in graded-index fiber. Fig. 2.11 shows the schematic diagram of a step-index fiber.

Fig. 2.11: Schematic diagram of a typical step-index fiber, n_{co} and n_{cl} are the refractive indices of the core and cladding, respectively [69].

Fig. 2.12: Schematic diagram of three types of optical fibers [69].

Optical fibers come in two main types [69]. Single-mode fiber has a small core with a diameter around $8\mu\text{m}$ that forces the light waves to stay in the same path, or mode. This keeps the light signals going farther before they need to be beefed up, or amplified. Most long-distance, or long-haul, fiber optic telephone lines use single-mode fiber. The second type, called multimode fiber, has a much larger core with a diameter around $65\mu\text{m}$. This gives light waves more room to bounce around inside as they travel down the path. The extra movement eventually causes the pulses to smear, losing part of the information. Fig. 2.12 shows the schematic diagram of single mode step-index fiber, multimode step-index fiber and multimode graded index fiber.

2.3.1.2 Guiding Mechanism

An optical fiber consists of two different types of highly pure, solid glass that are mixed with specific elements, called dopants, to adjust their refractive indices [69]. The difference between the refractive indices of the two materials causes most of the transmitted light to bounce off the cladding and stay within the core. The critical angle requirement is met by controlling the angle at which the light is injected into the fiber. Two or more layers of protective coating around the cladding ensure that the glass can be handled without damage. The principle of total internal reflection within a fiber core is illustrated in Fig. 2.13. The core has a higher refractive index than the cladding, allowing the beam that strikes that surface at less than the critical angle to be reflected. The second beam does not meet the critical angle requirement and is refracted.

Fig. 2.13: Principle of total internal reflection [69].

2.3.2 Biochemical sensing applications

Although different optical techniques could be used in biochemical sensors, it is the optical fibers that make their application in biochemical sensor development more practical [4]. It is usually said that application of optical fibers enables the scientist “to bring the spectrometer to the sample”. In fact, optical fibers are simply a platform which can be used in combination with different types of optical techniques, e.g. absorption, fluorescence, surface-enhanced Raman, surface plasmon resonance (SPR), etc. The great success of fiber-optic biochemical sensors is because they can be used to tackle difficult measurement situations where use of conventional optical biochemical sensors is not appropriate. For example, optical fibers can be used to transmit light over long distances and the bioreceptor need not to be in intimate contact with the optical fibers, enabling a wider range of non-invasive configurations. By using different multiplexing techniques, such as wavelength division multiplexing (WDM), time division multiplexing (TDM) or

spatial division multiplexing (SDM), it is able to achieve multiple analytes determinations.

Fig. 2.14: Evanescent wave biochemical sensor using partially clad fiber [3]. d_p is penetration depth.

Total internal reflection is the guiding mechanism of optical fibers. However, although the incident light is totally internally reflected, the intensity does not abruptly decay to zero at the interface [2]. Instead, a small portion of light penetrates the ambient medium, e.g. analytes solutions. This electromagnetic field is called evanescent wave, which has an intensity that decays exponentially with the distance. The penetration depth (d_p) is defined as the distance when the electric field amplitude falls to $1/e$ or its value at the interface [2]. The penetration depth increases with lower refractive index contrast at the interface and is also a function of the wavelength and the angle of incidence [3]. The evanescent wave interacts with the analytes solutions, offering the possibility of utilizing various optical techniques, such as absorption, fluorescence, SPR.

In the case of a clad fiber-optic probe, the amount of evanescent power is related to the fraction of light power in the cladding region compared to the total power.

Alternatively, it can be examined by the fraction of a mode's power that propagates within the core, which is defined as [70]

$$\eta = \frac{\text{Power flow within the core}}{\text{Total power flow of the mode}} \quad (2.3)$$

Fig. 2.15: The fraction of modal power residing in the core for each of the first twelve modes as a function of V . The dashed curve is for the fundamental modes when $n_{co}=n_{cl}$ and V is fixed [70].

Fig. 2.15 shows the fraction of modal power residing in the core for each of the first twelve modes as a function of V . V is defined as $V^2=U^2+W^2$, or $V = k\rho\{n_{co}^2 - n_{cl}^2\}^{1/2}$. Each mode of the fiber has minimum power within the core at cutoff. In particular the TE_{0m} , TM_{0m} , HE_{1m} and HE_{2m} modes have zero power with the core, i.e. $\eta=0$. Far from the cutoff, i.e. $V\rightarrow\infty$, all modes have their power concentrated in the core, i.e. $\eta\rightarrow 1$.

The amount of evanescent power is related to the fraction (f_e) of light power, in the cladding region compared to the total power. It can be defined as [5]

$$f_e = \frac{\text{Power flow within the cladding}}{\text{Total power flow of the mode}} = 1 - \eta \quad (2.4)$$

According to Fig. 2.15, a crucial factor determining f_e is the V number of the fiber. Since η has a monotonous increment with V number, the fraction f_e increases with the decreasing V number. This could be achieving by reducing the refractive index contrast between n_{co} and n_{cl} or reducing the radius ρ . Consequently, in order to enhance the interaction of the evanescent wave with the sensing layer, optical fibers are designed as unclad, partially clad, and D-shaped forms. The D fibers are fibers in which the cladding from one-half of the fiber is removed, exposing that half to the sensing layer. A major problem is V-number mismatch between the cladded region and the uncladded region. This causes the light enters into the decladded regions, and cannot couple back into the core. Thus, light loss cannot be solved. Approaches used to reduce the V-number mismatch are based on decreasing the radius of the fiber. The various geometries used for this purpose are shown in Fig. 2.16.

Fig. 2.16 Schematic of untapered and tapered fiber. A) Fiber probe with cladding stripped away from core. B) Step-tapered core to create V-number match between sensing and cladded regions. C) Continuously tapered core to maximize excitation light at surface. D) Combination tapered core to reach a V-number match quickly and subsequently maintain maximum excitation light at the fiber surface [3].

Optical fibers, including the unclad or D-shaped forms, have been demonstrated as evanescent wave spectroscopic sensors in combination of the conventional optical techniques. The spectroscopic information can be on the IR or UV-visible absorption or the Raman spectroscopic transitions. Near-IR and FT-IR spectroscopic approaches have also been demonstrated by using silver halide fibers [71], uncladded chalcogenide fibers [72] and sapphire fibers [73]. Besides, there is also continuing effort to develop miniature SPR platforms based on optical fibers, which have already had the performance comparable to the bulk-optic SPR sensors. Long-period fiber Bragg gratings, which can be viewed as a combination of the optical fibers and one dimensional photonic crystal, have also been developed as a label-free biochemical sensor with the ability of real-time detection and the potential for multiplexing [53, 54].

2.3.3 Advantages and Disadvantages

The use of an optical fiber as a platform into a biochemical sensor results in several advantages, e.g. [4, 5]:

1. An enormous number of optical techniques are available for biochemical analysis.
2. Use of a longer-length fiber provides a gain in interaction length or surface area for multiple analyte detection. It is able to use different segments of the same optical fiber, by appropriate labeling, to probe different analytes, thus providing an opportunity for multianalyte detection.
3. Fibers have a multiplex capability. Because they can guide light of different wavelengths at the same time and in different directions, multiple analyte determinations or single-analyte monitoring in single locations can be performed with a single central unit.
4. They can be easily miniaturized at low cost, thus finding application for in-vivo measurements. For example, one can use minimally invasive optical biochemical sensing methods to measure *in vivo* blood flow, glucose content, and so on.

Some drawbacks of optical-fiber sensors can limit their performance and applicability. A major limitation in the performance is determined by the thickness of the cladding. In order to enhance the performance of the fiber-optic biochemical sensor, the cladding of the optical fibers is usually removed, which results in a high loss and fragility. Particularly, in fluorescence detection, the efficiency of coupling of fluorescence

emission from the surface back into the fiber increases with an increase in the V number or an increase in the thickness of the cladding. Therefore, a dilemma is met by choosing the thickness of the cladding in order to improve the performance of fluorescence biochemical sensor. This type of ‘dilemma’ could be avoided by enabling the fluorescence emission to occur at the end surface of the fiber core rather than on the outer surface of the fiber cladding. However, several advantages of the fiber-optic sensor, such as long interaction length or surface area for multiple analyte detection, cannot be realized in this configuration.

2.4 Photonic Crystal Fibers

2.4.1 Wave-guiding Mechanisms

Having mentioned the nomenclature, the categories of the PCFs are divided based on their optical property. PCFs can be divided into two modes of operation, according to their mechanism for confinement [13, 14]. Index-guiding PCFs have a core with a higher average index than the microstructured cladding, and can operate on the same index-guiding principle as conventional optical fiber. In addition, they can have a much higher effective-index contrast between core and cladding, and therefore can have much stronger confinement for applications in nonlinear optical devices [74], polarization-maintaining fibers [75, 76]. They can also have a much lower effective-index contrast between core and cladding, for example to create large-mode-area fibers with very high nonlinear threshold powers [77, 78]. Alternatively,

a "photonic bandgap" fiber can be properly designed to confine light in a lower-index core and even a hollow (air) core by photonic bandgaps created by the microstructured cladding. Bandgap fibers with hollow cores can potentially overcome the limits imposed by available materials, for example to create fibers that guide light in wavelengths for which transparent materials are not available [79]. Another potential advantage of a hollow core is that one can dynamically introduce materials into the core, such as a gas that is to be analyzed for the presence of some substance [8, 80, 81].

2.4.1.1 Index-guiding PCFs

The index-guiding regions for conventional step-index fibers and index-guiding PCFs are demonstrated in Fig. 2.17(a) and (b), respectively. Considering a conventional step-index optical fiber, the effective index of the core mode, which is defined as n_{eff} , have the value between n_{co} and n_{cl} , or $n_{cl} < n_{eff} < n_{co}$. In other words, the cladding can only support the propagation modes with $n_{cl} < n_{eff} < n_{co}$. Those with either $n_{eff} < n_{cl}$ is leaky and thus cannot be supported by the cladding. Moreover, as the cladding is made from homogeneous material, the refractive index of the cladding is invariant across the wavelength range, assuming the material dispersion is not considered. The difference between step-index optical fiber and index-guiding PCF is the microstructured cladding. The effective index of the microstructured cladding is no more a constant but shows a large dependence of the wavelength, which is clear from Fig. 2.17. The line representing the refractive index cladding is named as radiation line, which have the effective index of

n_{fsm} , where n_{fsm} is the effective index of the fundamental space-filling mode of the crystal structure. The index-guiding region is between the core line and the cladding line, or $n_{\text{fsm}} < n_{\text{eff}} < n_{\text{co}}$.

Fig. 2.17: Refractive indices of the core and cladding in (a) a step-index profile fiber and (b) index-guiding PCFs.

A qualitative explanation for the strongly wavelength dependent cladding index is illustrated in Fig. 2.18. From the figure a very simple behavior of the intensity distribution of difference wavelength in the cross-section is observed [82]. For short wavelength, more intensity will concentrate in the high index region, i.e., silica, so the average refractive index of the cladding is approaching the refractive index of silica. On the other hand, for long wavelength, there will be a lot of energy in the air holes. So the average refractive index of the cladding will be smaller than that of short wavelength.

Fig. 2.18: Intensity distribution in the cladding of PCF for (a) short wavelength and (b) long wavelength [82].

2.4.1.2 Photonic Bandgap Fibers

The index-guiding PCFs have their effective cladding index dependent on the wavelength, which differs from the conventional step-index fibers and exhibits numerous novel properties, such as endless single mode guidance. However, there is no difference in their guiding mechanisms. Therefore, index-guiding PCFs can be merely viewed as an extension of the conventional step-index fibers.

In contrary, the invention of PBGFs is a revolution during the progress of optical waveguides. In a PBGF, light with proper wavelength can be guided in a low-index core, which has the refractive index smaller than the effective cladding index. Fig. 2.19 shows a gap map of a photonic crystal cladding, where the black-shaded regions are those for bandgap guiding and n_{co1} , n_{co2} and n_{co3} represent three different core indices. Clearly, the bandgap guiding regions are below the line representing the effective cladding index. Therefore, the bandgap guiding can be realized when the refractive index of the core is smaller than that of the cladding or $n_{co} < n_{fsm}$. The effective index of each guiding mode thus satisfies $n_{eff} < n_{co} < n_{fsm}$ and within the black-shaded regions.

Fig. 2.19: Schematic gap map of a photonic crystal cladding. Black-shaded areas are bandgap guiding regions.

Another characteristic to be observed is the bandgap guiding regions are separated by several frequency intervals, in which light may not penetrate the structure. The physical explanation of these low transmission intervals is to be found in multiple scattering and wave interference phenomena within the periodic structure [13]. Considering a wave propagating at normal incidence to the 1D periodic structure as illustrated in Fig. 2.20, each of the layers cause a fraction of the wave to be reflected as a result of the refractive-index difference. For specific frequencies (the ones falling inside the low-transmission intervals indicated in Fig. 2.20(a), the optical-path differences of the reflected wavelets, along with the phase changes introduced at the layer boundaries; cause the reflecting wavelets to interfere constructively. Provided the materials are free of absorption, the 1D structure may, hence, exhibit a high reflection of light within these frequency intervals. While for other frequencies (the ones falling inside the high-transmission intervals), the reflecting wavelets are not in phase as shown in Fig.

2.20(b). Hence, the incident wave will transmit with slightly attenuated. The formation of bandgaps in the PBGFs is much more complicated than the 1D case, but has the same principle.

Fig. 2.20: For wavelength in bandgap (a): A wave incident on a bandgap material [1] partially reflects off each layers of the structure [2]. The reflected waves are in phase and reinforce one another. They combine with the incident wave to produce a standing wave [3] that does not travel through the material. For wavelength not in bandgap (b): At wavelength outside the bandgap [1], the reflected waves are out of phase and cancel out each other [2], the light propagates through the material with only slightly attenuated [3].

It is straightforward to say that the radiation line divides the diagram into two distinct guiding regions. Above the radiation line, the guiding mechanism is similar to that in conventional step index fiber and index-guiding is appropriate enough to address such guidance. Below the radiation line, light can be guided by the bandgap effects in the black-shaded regions. Therefore, the guiding mechanism is dependent on the refractive index of the core. As shown in Fig. 2.19 if $n_{co}=n_{co1} > n_{fsm}$, light is guided along the optical waveguide by index-guiding mechanism inside the grey-shaded regions. On the other hand, if $n_{co}=n_{co2} < n_{fsm}$, light is guided by photonic bandgap effects inside the black-shaded regions. If $n_{co}=n_{co3}$, light cannot be guided by either index-guiding mechanism or bandgap guiding mechanism. Besides, their difference also manifests in the transmission spectrum. The transmission spectrum of the PBG fiber is characterized by having several transmission windows which are defined as bandgaps, while an index-guiding PCF does not. Fig. 2.21 shows a transmission spectrum for a typical hollow-core PBGF [20].

Fig. 2.21: Transmission spectrum of a typical hollow-core PBGF [20].

2.4.2 Potential advantages

PCFs inherit the advantages of fiber-optic biochemical sensors. In addition, especially two features of the PCFs have encouraged their use within sensors [83]. One is the possibility of obtaining long interaction lengths between light propagating in the fiber and very small volumes of gasses or liquid positioned in the air holes. The other is the freedom in the design of the optical properties of the fibers. The optical field can hence probe aqueous solutions of biomolecules positioned in the air holes or biomolecules captured at the silica-air interface.

In particular, exploration of PBGFs for biochemical sensing applications would be likely to overcome the drawbacks of the conventional step-index fiber and provide several novel sensing techniques. As compared to conventional step-index fibers, PBGFs are more favorable for the biochemical sensing applications for two major reasons:

1. PBGFs, especially hollow-core PBGFs, could provide high overlap between the optical power and the analytes residing in the holey region, including the hollow core and the holes in the cladding. It has been demonstrated that more than 95% of the optical power is located in the hollow core, the holes of the cladding and not in glass [9]. This is more than 20 times larger than the conventional step-index fiber, which relies on the evanescent wave extending outside the fiber. It could greatly enhance the sensitivity of spectroscopic type fiber-optic sensors, including absorption, fluorescence, surface plasmon resonance and Raman. In addition, since there is no need to remove the cladding

of hollow-core PBGF, the device is expected to be more robust for sensing applications.

2. They can provide novel sensing techniques by utilizing the photonic bandgap effects. The locations of the photonic bandgaps, or transmission windows in the spectrum, are a function of the refractive index contrast between the cladding materials. Hence, changes in a photonic bandgap upon capture of the analytes can be used as an indicator. Modifications of the refractive index profile in such photonic bandgap fibers will shift the position of the transmission windows defined by the bandgaps. The detection can then be done through measuring the position of the bandgaps or by monitoring the intensity of a single-wavelength signal with a wavelength at a bandgap edge. This sensing mechanism can also be realized by using a polymer based PBGF. One of the advantages of polymer based fibers over silica ones is, that many biological substances are more compatible with polymers than with silica. The preparation of the air holes with the deposition of a sensor layer should be easier and hence more reliable and reproducible.

Another promising biochemical sensing technique is to design PBGFs biochemical sensors in combination of liquid crystals. Liquid crystals are characterized by exhibiting a relatively strong interaction between the constituting molecules. The solid surface presents immobilized chemical receptors that weakly bind molecules that form a LC phase to orient it in a well-defined direction [47-49, 84]. In addition, the receptors bind targeted analytes, such as enzyme-lecithin reaction, more strongly than they bind the molecules forming the LC. These interactions introduce a sometimes rather advanced orientation of a large number of molecules, mainly determined by the surface anchoring

conditions and by modifying the orientation of the surface aligned molecules, e.g. at the surface of a glass slide, a large number of molecules are forced to adjust to the orientation of these differently oriented molecules. The orientation of LCs is expected to alter the transmission spectrum, which can be utilized for biochemical sensor applications.

2.5 Numerical Analysis of Photonic Bandgap Fibers

2.5.1 Introduction

The propagation of electromagnetic field can be described by its electric and magnetic field vectors. The evolution of the electric and magnetic field vectors is governed by Maxwell's equations [70]. Mathematically, the propagation of light in the optical waveguide can be treated by solving the differential equations derived from Maxwell's equations with homogeneous boundary conditions. Furthermore, the simple geometries of the conventional waveguides like step-index fibers or slab waveguides enable an explicit expression for their mode fields, such as cosine and Bessel functions, etc. Therefore, when considering the modeling of photonic crystal fibers (PCFs), it would be natural to introduce the concepts from standard waveguide or fiber analysis. However, there are several reasons that preclude PCFs from sharing the same advantages in the modeling of conventional optical waveguides. Firstly, it is the complex nature of the cladding or core structure of PCFs that does not allow for the direct use of single analytical expression for the mode fields. Secondly, the high index contrast nature between silica and air, for

example, requires full-vector treatment of the mode fields. Alternatively, in order to be able to design and accurately predict the properties of PCF structures, numerical techniques, such as plane wave method (PWM) and beam propagation method (BPM), must be applied.

2.5.2 Fundamentals

2.5.2.1 Maxwell's Equations

An electromagnetic field in space is described classically by two field vectors, $\mathbf{E}$ and $\mathbf{H}$, called the electric vector and magnetic vector, respectively. To include the effect of the field on matter, it is necessary to introduce a second set of vectors, $\mathbf{D}$ and $\mathbf{B}$, called the electric displacement and the magnetic induction, respectively. These vectors are related by macroscopic Maxwell's equations [85]

$$\nabla \times \mathbf{E}(\mathbf{r}, t) + \frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} = 0 \quad (2.1)$$

$$\nabla \times \mathbf{H}(\mathbf{r}, t) - \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} = \mathbf{J}(\mathbf{r}, t) \quad (2.2)$$

$$\nabla \cdot \mathbf{D}(\mathbf{r}, t) = \rho(\mathbf{r}, t) \quad (2.3)$$

$$\nabla \cdot \mathbf{B}(\mathbf{r}, t) = 0 \quad (2.4)$$

where $\mathbf{J}$ is the electric current density (amperes per square meter) and ρ is the electric charge density (coulombs per cubic meter).

These four equations are the basic laws of electricity and magnetism in their differential forms. The charge density ρ and electric current density $\mathbf{J}$ may be regarded as the sources of the electromagnetic radiation. However, for the source-free waveguide,

$\rho=0$ and $\mathbf{J}=0$. In addition, to allow a determination of the field vector from a given waveguide problem, these equations must be supplemented by relations that describe the effect of the electromagnetic field on materials. Particularly, in a linear medium, $\mathbf{D}=\epsilon\mathbf{E}$ and $\mathbf{B}=\mu\mathbf{H}$, where $\epsilon=\epsilon_r\epsilon_0$ and $\mu=\mu_r\mu_0$. Here, ϵ_0 and μ_0 are the permittivity and permeability of vacuum, respectively. ϵ_r and μ_r are the permittivity and permeability of the material, respectively. It is worth noting that ϵ_r and μ_r are tensors of rank 2. If the material medium is isotropic, these tensors reduce to scalars.

In general both $\mathbf{E}$ and $\mathbf{H}$ are complicated function of time and space. However, since the Maxwell's equations are linear, the time dependence can be separated out by expanding the fields into a set of harmonic modes [86]. It is convenient to represent each field vector as a complex function as a certain field pattern times a complex exponential:

$$\mathbf{H}(\mathbf{r},t) = \mathbf{H}(\mathbf{r})e^{j\omega t} \quad (2.5)$$

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r})e^{j\omega t} \quad (2.6)$$

Substituting these two equations into Eqs. (2.1), (2.2), (2.3) and (2.4), a phasor expression of EM field can be obtained

$$\nabla \times \mathbf{E}(\mathbf{r}) + j\omega\mu_0\mathbf{H}(\mathbf{r}) = 0 \quad (2.7)$$

$$\nabla \times \mathbf{H}(\mathbf{r}) - j\omega\epsilon_0\mathbf{E}(\mathbf{r}) = 0 \quad (2.8)$$

$$\nabla \cdot (\epsilon\mathbf{E}(\mathbf{r})) = 0 \quad (2.9)$$

$$\nabla \cdot \mathbf{H}(\mathbf{r}) = 0 \quad (2.10)$$

These equations describe the mode profiles of a given frequency. It is worth noting that only real parts of the expressions are the physical fields.

2.5.2.2 Full-vectorial wave equations

The Maxwell's equations described by Eqs.(2.7), (2.8), (2.9) and (2.10) are a set of coupled partial differential equations. These can be manipulated to yield differential equations which each of the field vectors satisfy a second-order differential equation. In the following, the discussion is limited in linear, lossless materials.

Applying a vectorial rotation operator $\nabla \times$ to Eq.(2.7), it is obtained [82]

$$\nabla \times \nabla \times \mathbf{E} - \epsilon_r k_0^2 \mathbf{E} = 0 \quad (2.11)$$

where $k_0 = \omega \sqrt{\mu_0 \epsilon_0}$ is the wave number in free space. Similarly, the magnetic field satisfies

$$\nabla \times \nabla \times \mathbf{H} - \frac{\nabla \epsilon_r}{\epsilon_r} \times \nabla \times \mathbf{H} - \epsilon_r k_0^2 \mathbf{H} = 0 \quad (2.12)$$

By using the identity

$$\nabla \times \nabla \times \equiv \nabla(\nabla \cdot) - \nabla^2 \quad (2.13)$$

The two wave equations in Eq. (2.11) and Eq.(2.12) can be further simplified as

$$\nabla^2 \mathbf{E} + \nabla \left(\frac{\nabla \epsilon_r}{\epsilon_r} \cdot \mathbf{E} \right) + \epsilon_r k_0^2 \mathbf{E} = 0 \quad (2.14)$$

$$\nabla^2 \mathbf{H} + \frac{\nabla \epsilon_r}{\epsilon_r} \times (\nabla \times \mathbf{H}) + \epsilon_r k_0^2 \mathbf{H} = 0 \quad (2.15)$$

These two vector equations are general and valid for all source-free EM problems.

Eqs. (2.14) and (2.15) are not the only way to represent the electromagnetic field in source-free medium. For example, $\mathbf{H}$ field can also be obtained in the following way. Divide the equation of (2.8), and then take the curl. Then use the equation to eliminate

$\mathbf{E}(\mathbf{r})$. The result in an equation entirely in $\mathbf{H}(\mathbf{r})$ [82]

$$\nabla \times \left(\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r}) \right) = k_0^2 \mathbf{H}(\mathbf{r}) \quad (2.16)$$

This is the master equation which can be directly solved in the well-know plane wave method for calculating band diagrams of photonic crystals or PCFs. Combined with the divergence equation in Eq.(2.10), $\mathbf{H}(\mathbf{r})$ can be completely determined. The electric field $\mathbf{E}(\mathbf{r})$ can be obtained by

$$\mathbf{E}(\mathbf{r}) = \left(\frac{-ic}{\omega \varepsilon(\mathbf{r})} \right) \nabla \times \mathbf{H}(\mathbf{r}) \quad (2.17)$$

2.5.2.3 Scalar wave equation

Scalar wave equation is derived when the refractive index contrast between the core and cladding is small, e.g. less than one percent. For such waveguide, the special differentiation of ε_r , or $\nabla \varepsilon_r$ is approximately zero. After taking this approximation, Eq. (2.11) becomes a scalar wave equation or Helmholtz equation, which can be written as

$$\left(\nabla_t^2 + k^2 - \beta^2 \right) \Psi = 0 \quad (2.18)$$

where Ψ represents either E_x, E_y, E_z, H_x, H_y and H_z .

PCFs are characterized by having a periodically arranged microstructure from two or more materials. If the refractive index contrast between these materials is small, the propagation of optical wave also satisfies the scalar wave equation.

2.5.3 Numerical Techniques

2.5.3.1 Overview of numerical techniques

In the development of the PCFs, the numerical modeling of the complex fiber structures become important, as the complex nature of the cladding does generally not allow for the direct use of methods from conventional fiber theory [87]. Especially for the photonic bandgap fibers (PBGFs), which guide light by photonic bandgap effect, the full vectorial nature of the electromagnetic waves must be taken into account. In order to address the issue of modeling, a number of numerical techniques have been developed and applied in understanding of these new fibers, including plane wave method (PWM) [88-91], beam propagation method (BPM) [92-95], finite difference method (FDM) [96-99], finite element method (FEM) [100-102], multipole method (MPM) [103, 104], localized functions method (LFM) [105, 106], Biorthonormal basis method (BBM) [107, 108], effective index method (EIM) [109], etc. For comparison, an overview of their advantages and disadvantages used for analysis and design of PCFs are listed in Table 2-1.

Method	Advantages	Disadvantages	Ref
Plane Wave Method (PWM)	+ Accurate + Numerically efficient + Simple to implement + Good agreement with experiments + Widespread approach	- Cannot treat loss - Cannot treat material dispersion	[88-91]
Beam Propagation Method (BPM)	+ Conceptually straightforward + Reliable method (well-tested) + Simple to implement + Can treat loss and material dispersion	- Relatively numerically inefficient	[92-95]
Finite Element Method (FEM)	+ Accurate + Reliable method + Can treat loss and material dispersion	- Complex definition of calculation mesh - Complex to implement	[100-102]
Finite Difference Method (FDM)	+ General approach + Can describe arbitrary structures + Reliable method	- Non-modal approach - Numerical intensive - Requires detailed treatment of boundaries	[96-99]
Multipole Method (MPM)	+ Describe effects of finite cladding region + Suited for symmetry structure + Leakage loss prediction	- Cannot analyze arbitrary cladding configuration	[103, 104]
Localized Functions Methods (LFM)	+ Solutions may be adapted to finite size structures + May describe random hole distributions	- Needs great care on result interpretation - Complex method - Inefficient PBG analysis	[105, 106]
Biorthonormal Basis Method (BBM)	+ Vectorial mode repress + Flexible and efficient + Highly accurate	- Demanding formulations	[107, 108]
Effective Index Method (EIM)	+ Simple + Low computation time	- No polarization - Inaccurate modal - No PBG analysis	[109]

Table 2-1: Overview of advantages and disadvantages concerning different numerical methods for the analysis of PCFs [110].

Among these methods, PWM and BPM are chosen to solve the wave-guiding problems within our research scope. One of the advantages of having two completely different methods to solve the same problem is that comparing the results gives some confidence in their accuracy. In addition, since these two methods have complementary advantages, they can rescue each other if one of them encounters a difficulty in solving a particular problem [111]. Therefore, it seems natural to choose two methods that are as different as possible. This is quite the case between PWM and BPM method. In the following sections, some of the most widely used full-vectorial numerical techniques used in the investigation of PCF research and applications are highlighted, including PWM, BPM, FDM and FEM. Their corresponding major theoretical techniques are also described. In an attempt to paint a detailed picture of a potential PCF application, a brief explanation of the physics underlying each approach, as well as a comparative study of the strengths and weaknesses of each method is provided.

2.5.3.2 Plane Wave Method

The plane wave method (PWM) was the first theoretical method to accurately analyze photonic crystals and PCFs [89, 90]. The concept originated from the methods used for solving the Schrödinger equation to predict electric bandgaps inside the semiconductors and other solid-state crystals. It is fast for frequency-domain analysis of full-periodic photonic crystals and PCFs. In addition, defect modes in both photonic crystals and PCFs

can also be evaluated by plane wave methods with the aid of so-called supercell technique. Due to its relative simplicity and wide applicability, the PWM has been the preferred method for analysis of structures exhibiting PBG effects. In the following text, the PWM used for evaluation of PBGs in anisotropic material is presented. The PWM used in isotropic material can be simply derived from the anisotropic case.

The anisotropic materials considered here are uniaxial crystal and biaxial crystal, which are lossless and transparent in the visible or infrared regime [84]. The uniaxial material has two different principal-refractive indices known as ordinary-refractive index n_o and extraordinary-refractive index n_e , while the biaxial crystal has three different principal refractive indices, namely, $n_x \neq n_y \neq n_z$. The dielectric constant ε here is a tensor instead of a simple scalar. Now considering in the principle axis, the diagonal elements of ε can be given by [112]

$$\varepsilon(\mathbf{r}) = \begin{pmatrix} \varepsilon_{xx}(\mathbf{r}) & 0 & 0 \\ 0 & \varepsilon_{yy}(\mathbf{r}) & 0 \\ 0 & 0 & \varepsilon_{zz}(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} n_x^2(\mathbf{r}) & 0 & 0 \\ 0 & n_y^2(\mathbf{r}) & 0 \\ 0 & 0 & n_z^2(\mathbf{r}) \end{pmatrix} \quad (2.19)$$

The $\mathbf{H}$ field is chosen for evaluating the bandgap structure for the sake of simplicity, and the Maxwell's equations can be rewritten as

$$\nabla \times (\varepsilon^{-1}(\mathbf{r}) \cdot \nabla \times \mathbf{H}(\mathbf{r})) = \frac{\omega^2}{c^2} \mathbf{H}(\mathbf{r}) \quad (2.20)$$

where $\varepsilon^{-1}(\mathbf{r})$ is the inverse of $\varepsilon(\mathbf{r})$. As the dielectric distribution is periodic, the $\mathbf{H}$ field can be represented by an infinite series of plane waves according to the Bloch theory

$$\mathbf{H}(\mathbf{r}) = \sum_{\mathbf{G}} \sum_{\lambda=1}^2 h_{\mathbf{G},\lambda} \hat{\mathbf{e}}_{\lambda} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} \quad (2.21)$$

where $\mathbf{k}$ is the wave vector of the Brillouin zone of the lattice, $\mathbf{G}$ is a reciprocal-lattice vector, and $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ are orthogonal unit vectors which are both perpendicular to the wave vector $\mathbf{k}+\mathbf{G}$ as the $\mathbf{H}$ field must satisfy the equation $\nabla \cdot \mathbf{H} = 0$. The PWM expansion method operates in reciprocal space. The transition from the real space to the reciprocal space is shown in Fig. 2.22.

Fig. 2.22: (a) The real-space (b) The reciprocal space of a 2D periodic structure with a hexagonal symmetry. $\mathbf{R}_1$ and $\mathbf{R}_2$ are the primitive lattice vectors, Λ is the lattice size, $\mathbf{G}_1$ and $\mathbf{G}_2$ are the reciprocal lattice vectors, the grey-area is the first Brillouin zone, Γ , M and K are the symmetry points [82].

Similarly, the dielectric tensor can also be expressed in Fourier transformations

$$\varepsilon^{-1}(\mathbf{r}) = \sum_{\mathbf{G}} \varepsilon^{-1}(\mathbf{G}) e^{i(\mathbf{G}\cdot\mathbf{r})} \quad (2.22)$$

Where $\varepsilon^{-1}(\mathbf{G})$ is the Fourier coefficients of $\varepsilon^{-1}(\mathbf{r})$. Substituting Eq. (2.21) and Eq.(2.22) into Eq. (2.20), a linear matrix equation can be found to be

$$\sum_{\mathbf{G}',\lambda'} H_{\mathbf{G},\mathbf{G}'}^{\lambda,\lambda'} h_{\mathbf{G}',\lambda'} = \frac{\omega^2}{c^2} h_{\mathbf{G},\lambda} \quad (2.23)$$

where

$$H_{\mathbf{G},\mathbf{G}'}^{\lambda,\lambda'} = |\mathbf{k} + \mathbf{G}| |\mathbf{k} + \mathbf{G}'| \begin{pmatrix} \hat{\mathbf{e}}_2 \cdot \boldsymbol{\varepsilon}_{\mathbf{G},\mathbf{G}'}^{-1} \cdot \hat{\mathbf{e}}_2 & -\hat{\mathbf{e}}_2 \cdot \boldsymbol{\varepsilon}_{\mathbf{G},\mathbf{G}'}^{-1} \cdot \hat{\mathbf{e}}_1 \\ -\hat{\mathbf{e}}_1 \cdot \boldsymbol{\varepsilon}_{\mathbf{G},\mathbf{G}'}^{-1} \cdot \hat{\mathbf{e}}_2 & \hat{\mathbf{e}}_1 \cdot \boldsymbol{\varepsilon}_{\mathbf{G},\mathbf{G}'}^{-1} \cdot \hat{\mathbf{e}}_1 \end{pmatrix} \quad (2.24)$$

Where $\boldsymbol{\varepsilon}_{\mathbf{G},\mathbf{G}'}^{-1} = \boldsymbol{\varepsilon}^{-1}(\mathbf{G} - \mathbf{G}')$.

The matrix involved is Hermitian and positive definite, and can be solved by freely available LAPACK [113]. Although the wave equation is only solved for the $\mathbf{H}$ field, the corresponding $\mathbf{E}$ field solution can be solved by using

$$\mathbf{E}(\mathbf{r}) = \frac{1}{j\omega\boldsymbol{\varepsilon}(\mathbf{r})\varepsilon_0} \nabla \times \mathbf{H}(\mathbf{r}) \quad (2.25)$$

The above equations are derived for anisotropic photonic crystals and PCFs. The isotropic counterpart can be easily derived by considering $n_x=n_y=n_z$. The only difference is that $\boldsymbol{\varepsilon}_{\mathbf{G},\mathbf{G}'}^{-1}$ becomes a scalar.

The PWM incorporates both simplicity and viability in a rather difficult and complex problem. The result is a clear detailed mapping of the energy band diagram of almost any type of periodic arrangement. It is fair to say that no PCFs would have been delivered to date without the aid of PWM technique. In addition, by combining this method with simple group theory analyses, it is possible to investigate large classes of crystal structures for possible photonic bandgap production.

In spite of this, however, the PWM suffers from several disadvantages [89, 90]. Among these is the inability to efficiently study crystal containing materials with frequency dependent dielectric functions, such as metals, for example. The main problem stems from the facts that the PWM fixes k and searches for all the possible values of ω , a

process that becomes exceedingly difficult and time consuming if ϵ is frequency dependent. Furthermore, the PWM is best suited for handling perfectly periodic systems. When a crystal structure contains a defect or some kind of disorder, a supercell type of approach may be applied to model the effect on the photonic band diagram. This again is very costly in terms of the number of plane waves. Finally, while this type of approach provides a deep physical insight into the origins of the photonic gap and the parameters affecting it, the PWM loses complete sight of potential applications, as it cannot provide any information about the viability of potential application such as a cavity produced via a point defect, or the guidance capability of a PCF. However, it certainly paints a clear picture of an invaluable portion of the overall photonic crystal portrait.

2.5.3.3 Beam Propagation Method

Beam propagation method (BPM) is a very well known tool for modeling integrated and fiber optic photonic devices [94, 95, 101, 114-116]. The popularity of the BPM arises from the conceptually straightforward, which allows rapid implementation of the basic technique. In addition, BPM is the approach that is readily applied to complex geometries without having to develop specialized versions of the method. Also the BPM methods can deal with the dispersion, loss as well as mode coupling and conversion. In the following subsections, the basic ideas involved in the BPM as well as the main extensions to the technique are explained.

Fig. 2.23: A general z-invariant waveguide.

Fig. 2.23 shows a general z-invariant waveguide. Similar to the PWM, the anisotropic material considered here have ϵ , which takes the form of [94, 95, 114]

$$\epsilon(\mathbf{r}) = \begin{pmatrix} \epsilon_{xx}(\mathbf{r}) & 0 & 0 \\ 0 & \epsilon_{yy}(\mathbf{r}) & 0 \\ 0 & 0 & \epsilon_{zz}(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} n_x^2(\mathbf{r}) & 0 & 0 \\ 0 & n_y^2(\mathbf{r}) & 0 \\ 0 & 0 & n_z^2(\mathbf{r}) \end{pmatrix} \quad (2.26)$$

The vector wave equation for the electric fields can be described by

$$\nabla \times \nabla \times \mathbf{E} - \epsilon(\mathbf{r})k_0^2 \mathbf{E} = 0 \quad (2.27)$$

where $k_0 = \omega\sqrt{\mu_0\epsilon_0}$ is the wave number in free space. By using the identity

$$\nabla \times \nabla \times \equiv \nabla(\nabla \cdot) - \nabla^2 \quad (2.28)$$

The transverse components $\mathbf{E}_t$ satisfy

$$\nabla^2 \mathbf{E}_t + \epsilon(\mathbf{r})k_0^2 \mathbf{E}_t = \nabla_t(\nabla_t \cdot \mathbf{E}_t + \frac{\partial E_z}{\partial z}) \quad (2.29)$$

Considering $\nabla \cdot (\epsilon(\mathbf{r})\mathbf{E}_t) = 0$, Eq. (2.29) becomes

$$\nabla_t \cdot (\epsilon_t(\mathbf{r})\mathbf{E}_t) + \frac{\partial n_z^2}{\partial z} E_z + n_z^2 \frac{\partial E_z}{\partial z} = 0 \quad (2.30)$$

As the dielectric tensor of PCFs are invariant along z - direction, $\partial \varepsilon(\mathbf{r})/\partial z = 0$, and thus Eq. (2.30) becomes

$$\frac{\partial E_z}{\partial z} = -\frac{1}{n_z^2} \nabla_t \cdot (\varepsilon(\mathbf{r}) \mathbf{E}_t) \quad (2.31)$$

Substituting Eq. (2.31) into Eq. (2.29), the wave equation for the transverse electric fields can be found to be

$$\nabla^2 \mathbf{E}_t + \varepsilon_t(\mathbf{r}) k_0^2 \mathbf{E}_t = \nabla_t \left(\nabla_t \cdot \mathbf{E}_t - \frac{1}{n_z^2} \nabla_t \cdot (\varepsilon_t(\mathbf{r}) \mathbf{E}_t) \right) \quad (2.32)$$

Assume that

$$\mathbf{E}_t = \hat{\mathbf{E}}_t e^{-jn_{eff} k_0 z} \quad (2.33)$$

As $\hat{\mathbf{E}}_t$ is invariant along z direction, substitute Eq. (2.33) into (2.32) gives rise to [94, 95]

$$P_{xx} \hat{E}_x + P_{xy} \hat{E}_y = 0 \quad (2.34)$$

$$P_{yx} \hat{E}_x + P_{yy} \hat{E}_y = 0 \quad (2.35)$$

where

$$P_{xx} \hat{E}_x = \frac{\partial^2 \hat{E}_x}{\partial y^2} + \frac{\partial}{\partial x} \left(\frac{1}{n_z^2} \frac{\partial}{\partial x} (n_x^2 \hat{E}_x) \right) + (n_x^2 - n_{eff}^2) k_0^2 \hat{E}_x \quad (2.36)$$

$$P_{yy} \hat{E}_y = \frac{\partial^2 \hat{E}_y}{\partial x^2} + \frac{\partial}{\partial y} \left(\frac{1}{n_z^2} \frac{\partial}{\partial y} (n_y^2 \hat{E}_y) \right) + (n_y^2 - n_{eff}^2) k_0^2 \hat{E}_y \quad (2.37)$$

$$P_{xy} \hat{E}_y = \frac{\partial}{\partial x} \left(\frac{1}{n_z^2} \frac{\partial}{\partial y} (n_y^2 \hat{E}_y) \right) - \frac{\partial^2 \hat{E}_y}{\partial x \partial y} \quad (2.38)$$

$$P_{yx} \hat{E}_x = \frac{\partial}{\partial y} \left(\frac{1}{n_z^2} \frac{\partial}{\partial x} (n_x^2 \hat{E}_x) \right) - \frac{\partial^2 \hat{E}_x}{\partial x \partial y} \quad (2.39)$$

For the isotropic material, Eqs. (2.34) and (2.35) can be modified by considering $n_x=n_y=n_z$. Eqs. (2.34) and (2.35) can be solved by using a finite-difference method.

It has been pointed out that BPM provides a simple intuitive method of determining the modal spectrum and model profiles for complex waveguides. This method, especially beam propagation correlation method, has been extensively used in the studies of complex structures and that it is particularly well suited to compute mode evolution in waveguides that vary in the longitudinal direction and in geometries, where leaky modes are important. An example related to this type of problems is the analysis of grating structures. Therefore, BPM is the first considered numerical methods which is complementary with PWM.

2.5.3.4 Finite Difference Method

Due to the simplicity and easy implementation, the finite difference method (FDM) is another one of the most commonly used numerical methods for the boundary value eigenvalue problem [96-99]. It is based on a semi-local approximation of the partial derivative through low order Taylor series expansions. For example, the central difference approximation of the second derivative for the function F with the variable f can be derived easily [96-99]:

$$\frac{\partial^2 F}{\partial f^2} = \frac{2}{h_1 + h_2} \left(\frac{F^{i+1}}{h_1} - F^i \left(\frac{1}{h_1} + \frac{1}{h_2} \right) + \frac{F^{i-1}}{h_2} \right) + O(\Delta x_i^2) \quad (2.40)$$

$$\frac{\partial}{\partial f} \left(\frac{1}{n^2} \frac{\partial (n^2 F)}{\partial f} \right) = \frac{2}{h_1 + h_2} \left(F^{i+1} \frac{n_{i+1}^2}{h_2 n_{i+1/2}^2} - F^i \left(\frac{n_i^2}{h_2 n_{i+1/2}^2} + \frac{n_i^2}{h_1 n_{i-1/2}^2} \right) + F^{i-1} \frac{n_{i-1}^2}{h_1 n_{i-1/2}^2} \right) + O(\Delta x_i^2) \quad (2.41)$$

where the non uniform mesh size Δ_{i-1} , Δ_i , and Δ_{i+1} are used and n_i is the refractive index at the mesh i as shown in Fig. 2.24. The mesh distances are that $h_1 = (\Delta_{i-1} + \Delta_i)/2$ and $h_2 = (\Delta_i + \Delta_{i+1})/2$. The refractive indices at the mesh nodes are that $n_{i-1/2}^2 = (n_{i-1}^2 \Delta_{i-1} + n_i^2 \Delta_i)/2h_1$ and $n_{i+1/2}^2 = (n_{i+1}^2 \Delta_{i+1} + n_i^2 \Delta_i)/2h_2$.

Fig. 2.24: The 1D finite difference mesh [97, 99]

As mentioned early, all functions under the partial derivatives in the full-vector eigenvalue equations of Eqs. (2.34) and (2.35) are continuous and they are directly discretized by using the central difference approximations without any extra treatment at the dielectric interface of the waveguide. For example, the finite difference expressions of the wave equations of (2.34) and (2.35) can be expressed as follows [96-99]:

$$P_{xx} E_x = \frac{T_x^{i+1,j} E_x^{i+1,j} - T_x^{i,j} E_x^{i,j} + T_x^{i-1,j} E_x^{i-1,j}}{\Delta x^2} + n_{i,j}^2 k^2 E_x^{i,j} + \frac{E_x^{i,j+1} - 2E_x^{i,j} + E_x^{i,j-1}}{\Delta y^2} \quad (2.42)$$

$$P_{yy} E_y = \frac{T_y^{i,j+1} E_y^{i,j+1} - T_y^{i,j} E_y^{i,j} + T_y^{i,j-1} E_y^{i,j-1}}{\Delta y^2} + n_{i,j}^2 k^2 E_y^{i,j} + \frac{E_y^{i+1,j} - 2E_y^{i,j} + E_y^{i-1,j}}{\Delta x^2} \quad (2.43)$$

$$P_{xy}E_y = \frac{1}{4\Delta x\Delta y} \left(\left(\frac{n_{i+1,j+1}^2}{n_{i+1,j}^2} - 1 \right) E_y^{i+1,j+1} - \left(\frac{n_{i+1,j-1}^2}{n_{i+1,j}^2} - 1 \right) E_y^{i+1,j-1} - \left(\frac{n_{i-1,j+1}^2}{n_{i-1,j}^2} - 1 \right) E_y^{i-1,j+1} + \left(\frac{n_{i-1,j-1}^2}{n_{i-1,j}^2} - 1 \right) E_y^{i-1,j-1} \right) \quad (2.44)$$

$$P_{yx}E_x = \frac{1}{4\Delta x\Delta y} \left(\left(\frac{n_{i+1,j+1}^2}{n_{i,j+1}^2} - 1 \right) E_x^{i+1,j+1} - \left(\frac{n_{i+1,j-1}^2}{n_{i,j+1}^2} - 1 \right) E_x^{i+1,j-1} - \left(\frac{n_{i-1,j+1}^2}{n_{i,j-1}^2} - 1 \right) E_x^{i-1,j+1} + \left(\frac{n_{i-1,j-1}^2}{n_{i,j-1}^2} - 1 \right) E_x^{i-1,j-1} \right) \quad (2.45)$$

where

$$T_x^{j\pm 1,j} = \frac{2n_{i\pm 1,j}^2}{n_{i\pm 1,j}^2 + n_{i,j}^2} \quad (2.46)$$

$$T_y^{i,j\pm 1} = \frac{2n_{i,j\pm 1}^2}{n_{i,j\pm 1}^2 + n_{i,j}^2} \quad (2.47)$$

where the uniform meshes Δx and Δy are used for the sake of simplicity.

In order to facilitate numerical solution within a finite computation domain, proper numerical boundary conditions must be used. In this work, a popular perfectly matched layer (PML) boundary conditions at the edge of the computation window to reduce the computation effort without sacrifice for accuracy and the graded index averaging technique to improve the numerical accuracy. By substituting the above finite difference expressions into the wave equations of (2.34) and (2.35), a system of the linear equations is obtained:

$$M \begin{bmatrix} E_x \\ E_y \end{bmatrix} = (kn_{eff})^2 \begin{bmatrix} E_x \\ E_y \end{bmatrix} \quad (2.48)$$

where k is the propagating constant in free space, n_{eff} is the complex modal effective index, and M is a band matrix with the bandwidth $(4N_x+6)$ and dimension $2N_x \times N_y$, in which N_x and N_y are the numbers of meshes in x and y directions. The effective indices and mode profiles can be obtained by using some eigenvalue solvers, such as the shifted inverse power method, the Lanczos method, and the Arnoldi method.

There are some rather serious drawbacks of this method [96-99]. Firstly, the band structure calculations performed using this method are not preferred due to the need of extremely careful choice of the initial fields, as well as the necessity of high time resolution for the ability to distinguish between parasite pulses originating from the numerical space termination at the boundaries and the actual signal. Moreover, this method can not effectively treat lossy and gain media. The reason stems from the infinitesimal extent of the spatial parameters describing these materials. For example, when modeling a lossy metal, one must incorporate an extremely fine spatial grid to account for the infinitesimal metallic skin-depth. This immediately magnifies the time and memory requirements of the algorithm, rendering it practically useless for such cases.

2.5.3.5 Finite Element Method

The finite element method (FEM) is extremely general as it allows the treatment of a large class of partial differential equations, including nonlinear problems and without any limitation on the geometry involved [100-102]. Contrary to PWM which is particularly

suited for periodic dielectric structure, FEM is an all-purpose method. The price to pay is, of course, a higher computational cost together with an associated reduction in speed.

The FEM divides the cross section of the fiber into a patch work of triangular elements which can be of different sizes, shapes, and refractive indices. In this way, any kind of geometry of the holes in PCF can be taken into account with high accuracy. An example of the discretized cross-section of a PCF is demonstrated in Fig. 2.25.

Fig. 2.25: An example of detail meshes which discretize the cross-section of a PCF [87].

The following eigenvalue algebraic problem can thus be written as

$$([A] - n_{eff} [B])\{h\} = 0 \quad (2.49)$$

The eigenvector $\{h\}$ and the eigenvalue provide, respectively, the full vector magnetic field distribution on the cross section and the effective index of the mode. Chromatic dispersion of the silica can be taken into account in Eqs. (2.16) and (2.49) by calculating through the Sellmeier equation. Starting from the knowledge of the effective index versus

the wavelength obtained by solving Eq.(2.49), the inverse of the group velocity and the group velocity dispersion parameter can be obtained by using finite difference formulas. The matrices $[A]$ and $[B]$ are sparse, allowing an efficient resolution of the equation by means of high performance algebraic solvers. In this work, high-order edge elements are used to provide very accurate effective-index values, and to avoid spurious modes in the guided-mode spectrum. In particular the considered formulation employs six tangential unknowns and two facial ones for each triangular element. In order to save computational efforts, structure symmetries can be exploited for the numerical simulations.

The disadvantage of FEM is the requirement of complex definition of calculation meshes [100-102]. In addition, challenging problems would certainly be the determination of losses in the case of leaky modes and also the study of nonlinear PCFs.

2.6 Chapter Summary

In this chapter, the basic optical principles and the various techniques utilized in biochemical sensing are described. The fundamentals for the propagation of light in the optical waveguide have been described. The scalar wave approximation is strictly valid for the small refractive index contrast situation. As PCFs are characterized by having high index contrast, the vectorial effects must be taken into consideration. In addition, due to the complex nature of the structure of PCFs, the Maxwell's equations cannot be solved analytically. Therefore, various numerical methods have been compared in terms

of accuracy, efficiency, applicability and etc. Fiber-optic biosensors, which combine the various optical techniques and advantages of optical fibers, have been the most widely studied optical biosensors for more than over two decades. The use of optical fibers in biosensors takes advantage of the versatility of these components. System configuration can be changed to suit the user's configuration. Shortened fibers can be used in sensors designed for portability, while fibers of extended length allow assays to be performed in remote or hazardous locations. A key disadvantage of evanescent wave systems is the lack of power within evanescent wave. Although the thickness of the cladding could be greatly reduced in order to increase the power within evanescent wave, it suffers the cost of fragility. More in particular, it increases the difficulty for coupling the emitted fluorescence back into the fiber. The emergence of the PCFs provides a solution to enhance the strength of evanescent wave, but without the need for removing the cladding. More importantly, novel sensing techniques could be realized by utilizing the bandgap shift of the PBGFs due to the presence of the biomolecules.

In the following chapters, the theoretical models of two kinds of PBGFs, isotropic PBGFs and anisotropic PBGFs are discussed in Chapter 3 and Chapter 4, respectively. In Chapter 5, several PBGFs based biochemical sensors are experimentally demonstrated with the aid of these theoretical models.

Chapter 3

Isotropic Photonic Bandgap Fibers

3.1 Introduction

In this chapter, a new theoretical model of the refractive index effect on the gap formation in isotropic photonic bandgap fibers (PBGFs) is presented. The theoretical model is further proved by numerical results. The isotropic PBGFs are grouped according to core and cladding compositions. The first category of PBGFs has a solid core with high-index inclusions in the cladding; the second has a hollow-core with low-index inclusions in the core and cladding.

The optical properties of the isotropic PBGFs are determined by the geometry and refractive index profile [117]. Any variation of the refractive index of the high-index or low-index inclusions is expected to shift the transmission windows, which are defined by the bandgaps. The detection can then be done through measuring the positions of the bandgaps or by monitoring the intensity of a single-wavelength signal with a wavelength at a bandgap edge. Although this concept is simple, one difficulty that arises is to determine the relationship between the variation of the refractive index profile and the shifts of the transmission windows. Numerical methods, such as plane wave method (PWM) or beam propagation methods (BPM), have the benefit of providing accurate

solution. However, the simulation time, which takes from one or two hours to several days, is always a burden. In addition, qualitative understanding is not easy to be obtained from just observing the simulation results. To address the above shortcomings, analytical models are derived, which utilizes the knowledge of the modal properties of step-index fibers as well as the scalar wave approximation of Maxwell's equations.

In particular, for solid-core PBGFs with high-index inclusions, an explicit expression is derived based on the antiresonant reflecting optical waveguide (ARROW) model [118-120], together with the modal properties of a step-index fiber. On the other hand, for the hollow-core PBGFs with low-index inclusions, the derivation is performed by analyzing the scalar wave equation.

3.2 Solid-core photonic bandgap fibers

3.2.1 Antiresonant reflecting optical waveguide model

Fig. 3.1: Solid-core PBGF with its air holes arranged in a triangular lattice. Black regions represent high-index inclusions, where $n_a > n_b$.

ARROW was named by Duguay et al., which attributed the guidance to the antiresonance of the high-index layer (analogous to a Fabry-Perot resonator) placed adjacent to the low-index core [121]. This geometry differs from the traditional total internal reflecting waveguide, which requires a high-index core to guide light. Besides that, one of the key signatures in the transmission spectrum of an ARROW waveguide is an approximately periodic spectral response with the wavelength. The model states that the resonant condition of an individual high-index layer determines the guidance in the low-index core. When the high-index cladding layers are in resonance with the core mode, light extends outwards by the high-index cladding layers. When the layers are in antiresonance with the core mode, light is reflected back from the high-index cladding layers and thus confined in the low-index core.

Although the traditional ARROW model was used to analyze the slab-type waveguides, it is possible to be extended for the explanation of guiding mechanism of the solid-core PBGFs [116, 119, 122]. The spectral response with wavelength can be appreciated by considering each high-index cylindrical rod (cladding layer), according to the ARROW model. One critical factor that determines the spectral properties of solid-core PBGFs is the cutoff wavelengths of the guiding modes. For a step-index fiber, the effective index of the core mode is approximately equal to that of silica at cut-offs. Therefore, at the cutoff wavelengths of the modes of the high-index inclusions, the entire solid-core PBGFs become effectively transparent [123, 124]. This certainly induces transmission minima in the transmission spectrum. As the wavelengths leave the cutoff

wavelengths and decrease, the effective index of the core mode of the high-index inclusions starts to increase. As a consequence, light begins to experience scattering by those high-index inclusions, which leads to the formation of transmission windows.

In the weakly guiding conditions, the eigenmodes of a step-index fiber can be classified as LP_{ml} modes, where m is the order of the mode, and the second subscript l denotes the l th root of the eigenvalue equation [70]. LP_{0l} modes are twofold degenerate (corresponding to the two polarization directions) whereas modes with higher l are four fold degenerate. An exact solution of the problem reveals that each LP_{ml} multiplet with $m > 1$ consists of two closely spaced, doubly degenerate, eigenmodes, denoted $EH_{m-1,l}$ and $HE_{m+1,l}$, whereas the LP_{1l} modes consist of TE_{0l} , TM_{0l} and HE_{2l} modes. The LP_{0l} states in this terminology are HE_{1l} hybrid modes [122]. The modal cutoff conditions for the LP_{ml} mode can thus be written as

$$J_{m-1}(k_l d/2)_l = 0 \quad (3.1)$$

where $k_l = \frac{2\pi}{\lambda} \sqrt{n_a^2 - n_b^2}$ and l represents the l th root of Bessel function $J_{m-1}(x)$. Correspondingly, the explicit expression of the cut-off wavelength λ_{ml} of LP_{ml} mode can be described as

$$\lambda_{ml} = \frac{\pi d}{j_{m-1,l}} \sqrt{n_a^2 - n_b^2} \quad (3.2)$$

where $j_{m-1,l}$ is the l th zero of Bessel function $J_{m-1}(x)$.

Fig. 3.2: Plot of Bessel function of the first kind, $J_\alpha(x)$, for integer orders $\alpha=0, 1, 2, 3$.

Fig. 3.2 shows a plot of Bessel function of the first kind, $J_\alpha(x)$, for integer orders $\alpha=0, 1, 2, 3$. Although the solutions of Bessel functions cannot be represented by explicit functions, they can be approximated by using the asymptotic forms of $J_{m-1}(x)$ for positive integral m . Particularly, for large arguments $x \gg |(m-1)^2 - 1/4|$, they become [125]:

$$J_{m-1}(x) \rightarrow \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{(m-1)\pi}{2} - \frac{\pi}{4}\right) \quad (3.3)$$

Observing Eq.(3.3), it is found that $J_{m-1}(x)$ and $J_{m+1}(x)$ share the same solutions, when $x \gg |(m-1)^2 - 1/4|$. In other words, the cutoff wavelengths of $LP_{m,l}$ modes coincide with that of $LP_{m+2,l}$ modes, which can be validated from Fig. 3.2.

3.2.2 Numerical analysis and verification

Fig. 3.1 shows the structure of solid-core PBGF used in the simulation. After the filling process, the solid-core PBGF has a triangular arrangement of high-index inclusions of

index n_a embedded in a silica material of index n_b or $n_a > n_b$. The diameters of the high-index inclusions and their spacing are d and Λ , respectively. In order to determine the transmission windows for guiding light, PWM was used to evaluate the bandgap structure of the infinite photonic crystal (PC) cladding. The parameters are defined as $n_b=1.45$, $n_a=1.64$ and $d/\Lambda=0.59$.

Fig. 3.3: Enlarged gap map with normalized wavelength ranging from 0.125 to 0.3. Inset figure: Full gap map of the photonic crystal cladding.

Fig. 3.3 represents the gap map of the PC cladding. In order to have a clear identification of the cut-offs of corresponding modes of an individual high-index inclusion, the higher order bandgaps with normalized wavelength ranging from 0.125 to 0.3 are enlarged; while the full gap map is demonstrated in the inset figure. The wavelength ranges of the transmission bands or bandgaps in a silica core can be easily

identified, which are the spans where the core line $n_{eff}=1.45$ crosses the gap regions. These transmission bands are separated by the stop bands, which are the spans where the core line crosses the white region. The numerical labels used in the figure represent the orders of LP_{ml} modes. In the weakly guiding approximation, the eigenmodes of a step-index fiber can be classified as LP_{ml} modes. Particularly, LP_{0l} modes are HE_{1l} modes and LP_{1l} modes comprise TE_{0l} , TM_{0l} and HE_{2l} modes. The dot lines represent the modal cut-offs of LP_{0l} and LP_{1l} modes and the dash lines represent the modal cut-offs of higher order modes. The first thing to notice about the band structure is that not only LP_{0l} and LP_{1l} modes but also higher order modes LP_{ml} ($m \geq 2$) take part in the formation of stop bands. It should be noted that LP_{2l} derived stop bands are immersed in the much broader $LP_{0, l+1}$ stop bands. However, the stop bands show differences on the widths. The LP_{ml} ($m < 3$) related stop bands are quite broad, whereas the LP_{ml} ($m \geq 3$) cut-offs lead to narrow stop bands. This can be rationalized when considering the link between the properties of a single high-index inclusion at cut-off and the properties of entire PC cladding consisting of a silica background with periodic arranged high-index inclusions. For a single high-index inclusion, the effective index of the core mode is approximately equal to that of silica at cut-offs. Therefore, when the operating wavelengths are at the cutoff wavelengths, the entire waveguide becomes effectively transparent. The whole waveguide becomes lossy and transmission minima manifest in the transmission spectrum. When the wavelength reduces, light can be scattered by those high-index inclusions. Transmission windows can thus appear in the transmission spectrum. For the

lower order mode such as LP_{0l} and LP_{1l} modes, the increases of effective indices are quite slow. Thus, LP_{0l} and LP_{1l} related stop bands are relatively broad. As the order of modes increases, the change of effective indices speeds up greatly. This requires increasingly narrow wavelength ranges to change from stop bands to transmission bands. As a result, LP_{ml} ($m \geq 3$) related stop bands become extremely narrow and even splitting as observed from Fig. 3.3.

3.3 Hollow-core photonic bandgap fibers

3.3.1 Refractive index scaling law

Fig. 3.4 shows the cross section of a typical hollow-core PBGF. It consists of an air core which is surrounded by five rings of circular air holes. The circular air holes are arranged in a triangular lattice. The black region is for air holes, while the white region is for silica. The background material is assumed to be made of silica and it has the refractive index of 1.45.

Fig. 3.4: Hollow-core PBGF with its air holes arranged in a triangular lattice. Black regions represent air.

Two parameters of interests for the hollow-core PBGF are the positions and bandwidths of the bandgaps. These two parameters are functions of the geometry of the fiber and the index contrast between fiber materials, i.e., silica and low index material. The modification of the refractive index of the low index material can change the locations and bandwidths of the bandgaps simultaneously. However, there is no explicit expression to describe the relationship between the changes of the positions or bandwidths of the bandgaps and the variation of the refractive index of the circular holes. This thus imposes the difficulties on the design and analysis of the performance of the biochemical sensors by the use of hollow-core PBGFs.

To derive an explicit expression, a certain kind of approximation must be made in order to solve the Maxwell equation. A weakly-guiding approximation or scalar approximation can be made, assuming the refractive index contrast is small [126]. After taking this scalar approximation, the Maxwell equation can be reduced into a scalar equation, i.e.

$$\nabla_t^2 \varphi = (\beta^2 - k_0^2 \varepsilon(x, y)) \varphi \quad (3.4)$$

where $k_0 = \omega/c = 2\pi/\lambda$ is the wave vector, $\varepsilon(x, y)$ is the transverse dielectric constant profile, β is the propagation constant and φ denotes either E_x , E_y , E_z , H_x , H_y or H_z .

The transverse dielectric constant profile can be described in terms of normalized transverse coordinates $X=x/\Lambda$ and $Y=y/\Lambda$, which is given by

$$\varepsilon(X, Y) = \varepsilon_b + (\varepsilon_a - \varepsilon_b)g(X, Y) \quad (3.5)$$

where

$$g(X, Y) = \begin{cases} 0 & \text{low index regions} \\ 1 & \text{high index regions} \end{cases}$$

The corresponding wave equation can thus be rewritten as

$$\frac{\partial^2 \Psi}{\partial X^2} + \frac{\partial^2 \Psi}{\partial Y^2} + (v^2 g(X, Y) - w^2) \Psi = 0 \quad (3.6)$$

where $v^2 = \left(2\pi \frac{\Lambda}{\lambda}\right)^2 (n_b^2 - n_a^2)$ and $w^2 = \left(2\pi \frac{\Lambda}{\lambda}\right)^2 (n_{eff}^2 - n_a^2)$.

The refractive index scaling law can be described as follows: if n_a or n_b are varied, the scalar field distribution ψ can be kept unchanged, supposing that the normalized

wavelength λ/Λ is adjusted so as to keep the value v and w invariant. In particular, the locations of the transmission windows after the hollow-core PBGF is filled with aqueous solution can be estimated by considering the invariant v . The invariant v also yields

$$\frac{\lambda}{\Lambda} = C \cdot \sqrt{(n_b)^2 - (n_a)^2} \quad (3.7)$$

where C is a constant which is determined by the fiber structure. This simple formula provides a simple tool for use in the design and analysis of PBGF based biosensors. Supposing that the bandgaps originally at a wavelength λ_0 for an air-guiding hollow-core PBGF with $n_a=1$, after the fiber is filled with aqueous solution with $n_a=n_r$, it shifts to a new wavelength λ , which is given by

$$\lambda = \lambda_0 \left(\frac{n_b^2 - n_r^2}{n_b^2 - 1} \right)^{\frac{1}{2}} \quad (3.8)$$

3.3.2 Numerical Analysis and Verification

Inasmuch the tunability is dependent on wavelength shift of the photonic bandgap edge (PBE) with respect to the change of refractive index, in the following, the variation of the primary photonic bandgap (PBG) region with respect to the modification of the refractive index of n_a and air-filling fraction of f will be presented. The air-filling fraction is the total hole volume fraction which is equal to $\pi d^2/(2\sqrt{3}\Lambda^2)$ for the circular holes. The knowledge of the primary bandgap was obtained by a full-vectorial PWM method in which primitive basis vectors were used, and the number of plane waves was set to be 256×256 . After the location of the bandgap was obtained, the corresponding transmission

spectrum was evaluated by a full-vectorial BPM method. This was done by launching a Gaussian beam in the center of the core with the width equal to that of the core and the propagation length was $2^{11}\mu\text{m}$. The analytical results were evaluated by Eq.(3.7). The higher order PBGs will not be taken into account due to their narrow bandwidths and far away from the primary band.

Fig. 3.5 shows the transmission window, i.e. bandgap, for the fiber with air fraction of $f=0.7$ and water is filled into the circular holes. The refractive index of water is 1.33. The distance between the adjacent holes is chosen to be $\Lambda=3.6\mu\text{m}$ in order to adjust the central wavelength of the transmission window around 1550nm. The transmission window spans from $1.35\mu\text{m}$ to $1.65\mu\text{m}$ which represents the primary bandgap.

Fig. 3.5: Transmission spectrum for a PBG fiber filled with water. Inset figure: Shaded regions are gap regions [127].

Fig. 3.6: (a) Transmission spectra for different index profiles within the circular holes. (b) Wavelength shifts of two edges of the transmission window [127].

To evaluate the validity of the refractive index scaling law, the transmission spectra for different index profiles within the holes are shown in Fig. 3.6(a). Taking the 3-dB transmission points in the rising edge and falling edge of the transmission window as a reference, the corresponding wavelength shifts of two edges of the transmission window are illustrated in Fig. 3.6(b). It shows that the transmission window has a blue shift and the corresponding bandwidth shrinks with the increase of the refractive index. For the fiber which is shown in Fig. 3.4 with a pitch of $3.6\mu\text{m}$, the rising edge and falling edge of the transmission window shifts from 1355nm to 563nm and from 1630nm to 677.7nm, respectively, when the refractive index increases from 1.33 to 1.43.

Fig. 3.7 shows the variations of the bandgaps with different air-filling fractions as the refractive index changes when the binding of the biomolecules occurs. For comparison, the pitches for the PBG fibers with three air-filling fractions are the same values which are $3.6\mu\text{m}$. It is clear from Fig. 3.7, the wavelength shifts of the bandgaps show a good agreement with the refractive index scaling law. When the pitches are same, the hollow-core PBGFs with less air-filling fractions tend to have large wavelength shifts.

Fig. 3.7: Variations of the bandgaps with different air-filling fractions as the refractive index changes [127].

3.3.3 Vectorial effects on the bandgap formations

Similar to (2.34) and (2.35), a pair of coupled equation for $H_x(x, y)$ and $H_y(x, y)$ can be given by [95, 115]

$$(\nabla_t^2 - \beta^2 + k_0^2 \varepsilon(\mathbf{r})) H_x = P_{xx} H_x + P_{xy} H_y \quad (3.9)$$

$$(\nabla_t^2 - \beta^2 + k_0^2 \varepsilon(\mathbf{r})) H_y = P_{yy} H_y + P_{yx} H_x \quad (3.10)$$

where

$$P_{xx} H_x = \frac{1}{\varepsilon(\mathbf{r})} \frac{\partial \varepsilon(\mathbf{r})}{\partial y} \left(\frac{\partial H_x}{\partial y} \right)$$

$$P_{yy} H_y = \frac{1}{\varepsilon(\mathbf{r})} \frac{\partial \varepsilon(\mathbf{r})}{\partial x} \left(\frac{\partial H_y}{\partial x} \right)$$

$$P_{xy} H_y = -\frac{1}{\varepsilon(\mathbf{r})} \frac{\partial \varepsilon(\mathbf{r})}{\partial y} \left(\frac{\partial H_y}{\partial x} \right)$$

$$P_{yx}H_x = -\frac{1}{\varepsilon(\mathbf{r})} \frac{\partial \varepsilon(\mathbf{r})}{\partial x} \left(\frac{\partial H_x}{\partial y} \right)$$

The vector waves may be decomposed into TE (y -polarized transverse $\mathbf{E}$ -field and x -polarized $\mathbf{H}$ -field) and TM (y -polarized transverse $\mathbf{E}$ -field and x -polarized $\mathbf{H}$ -field) waves. As seen from Eqs.(3.9) and (3.10), the discontinuities of the dielectric constant $\varepsilon(\mathbf{r})$ across the refractive index interface along x and y directions are responsible for the polarization dependence (P_{xx} and $P_{yy} \neq 0$) and coupling effect (P_{xy} and $P_{yx} \neq 0$). If the coupling effect between two polarizations H_x and H_y is weak, the coupling terms P_{xy} and P_{yx} in Eqs.(3.9) and (3.10) can be neglected and the two polarizations can be treated independently by using semi-vector eigenvalue equations which are given by [95]

$$\left(\nabla_t^2 - \beta^2 + k_0^2 \varepsilon(\mathbf{r}) \right) H_x = P_{xx} H_x \quad (3.11)$$

$$\left(\nabla_t^2 - \beta^2 + k_0^2 \varepsilon(\mathbf{r}) \right) H_y = P_{yy} H_y \quad (3.12)$$

Eqs.(3.11) and (3.12) can be further simplified by neglecting the polarization dependence terms P_{xx} and P_{yy} if the structures are weakly guiding and/or the polarization dependence is not an issue. The governing equation for the polarization independence approximation, i.e. scalar wave approximation, can be given by [115]

$$\left(\nabla_t^2 - \beta^2 + k_0^2 n^2 \right) \Psi = 0 \quad (3.13)$$

where Ψ stands for either H_x or H_y .

By using the plane wave method, the photonic band structures can be evaluated and shown in Fig. 3.8(a), (b) and (c) from the scalar wave approximation, semi-vector

approximation and full-vector equation, respectively. The number of plane waves was set to be 121×121 . The air-filling fraction was assumed to be $f=0.7$. n_a and n_b were the refractive indices of the hole regions and background regions and were chosen to be 1 and 1.45, respectively. β were chosen to be 10. Two PBGs will be considered here, including the primary PBG and the secondary PBG. Since the vectorial effects play different roles in the formation of these two PBGs, the analysis is general and can be applied in the other high order PBGs.

Firstly, the formation of the primary PBG is investigated. As shown in Fig. 3.8(a), the primary PBG is able to be formed by the index contrast perturbation without considering the vector effects. Since two polarizations are degenerate in the scalar approximation, each band represents two photon states. However, this degeneracy will be splitted by considering the polarization dependence, i.e. the non-zero terms P_{xx} and P_{yy} in Eqs.(3.11) and (3.12). As shown in Fig. 3.8(b), the polarization dependence will shift all the bands upwards and thus results in the shift of the primary PBG. The width of the primary PBG is also narrowed by the polarization effects. Furthermore, the coupling effect, i.e. the non-zero terms P_{xy} and P_{yx} in Eqs.(3.9) and (3.10), accounts for the split of the degeneracy of the fifth and sixth bands at the Γ -point which in turn shrinks the primary PBG as shown in Fig. 3.8(c).

Fig. 3.8: Photonic band structures of (a) scalar wave approximation, (b) semi-vector approximation and (c) full-vector case. ($f=0.7$, $n_a=1$, $n_b=1.45$, $\beta=10$) [127]

The formation of the secondary PBG differs from the primary one. Under the scalar approximation as shown in Fig. 3.8(a), secondary PBG is unable to be formed due to the degeneracy of the 7th, 8th, 9th and 10th bands at the K-point in the Brillouin zone. The polarization dependence can only split the degeneracy of the 4th and 5th bands at the K-point for the TM waves; while the 4th and 5th bands for the TE waves are still degenerate in this case as shown in Fig. 3.8(b). Interestingly, the coupling between these two polarizations is able to split the degeneracy of the 4th and 5th bands for the TE waves and thus plays a central role in the formation of the secondary PBG which is shown in Fig. 3.8(c).

Fig. 3.9: Positions of PBGs on the low-index line vs. refractive index contrast. Shaded regions: full-vector PWM. Dashed lines: scalar PWM. ($n_b=1.45$, $n_a=1.45-\Delta n$) [127].

Since the vectorial effects are directly related to the refractive index contrast, the two PBGs will behave differently with the change of the refractive index contrast. The

primary and secondary PBGs on the low-index line are plotted against the refractive index contrast in Fig. 3.9. The low-index line represents $\beta=n_a k_0$, which is the air-line case for the air guiding, as demonstrated in the inset of Fig. 4.5. The shaded regions are these two PBGs which are evaluated by Eqs.(3.9) and (3.10), i.e. the full-vector PWM. The dashed lines are the PBEs which are evaluated by Eq.(3.7), i.e. the scalar wave approximation. This representation is same in the following figures. The results confirm that the primary PBG can exist for arbitrarily small refractive index contrast. Hence, the refractive index perturbation is responsible for the existence of the primary PBG. However, the secondary PBG can only exist for a large refractive index contrast when the polarization dependence and coupling effect are strong enough. Therefore, the scalar wave equation is unable to predict the existences of the PBGs which are formed by the vector effects. In addition, when the refractive index contrast is small, the primary PBG obeys the refractive index scaling law. The discrepancy in the large refractive index contrast is due to the polarization dependence and coupling effect which will narrow the primary PBG and shift its position.

Fig. 3.10: Locations of primary PBGs on the low-index line vs. refractive index contrast for different air-filling fractions. Shaded regions: full-vector PWM. Dashed lines: scalar PWM. ($n_b=1.45$, $n_a=1.45-\Delta n$) [127].

Besides refractive index contrast, the air-filling fraction is another factor that affects the polarization dependence and coupling effect and thus affects the formation of PBGs. Fig. 3.10 shows the variations of the location and width of the primary PBG on the low-index line with respect to the refractive index contrast for different air-filling fractions. It is worth noting that the results of the scalar PWM tend to be consistent with the results of the full-vector PWM when the air-filling fraction increases. This may come as a surprise, since the scalar wave approximation is normally used in the small air-filling fraction case. In the large air-filling fraction case, the structure tends to be uniform as a material with refractive index of n_a and thus the scalar wave approximation is valid. This is quite similar to the small air-filling fraction case where the structure tends to be uniform as a material with refractive index of n_b . Therefore, the scalar wave

approximation should be at least valid for the near-uniform structure and/or small refractive index contrast case.

The discussion can be further extended to the higher order PBGs. For the PBGs which are formed without the aid of vectorial effects, the scalar wave approximation gives reasonable prediction of the behavior of the PBGs. However, for the PBGs in which the vectorial effects are necessary in their formations, the scalar wave approximation is no longer valid.

3.4 Chapter Summary

Theoretical models have been developed to investigate the relationship between the refractive index and the locations of bandgaps. Two kinds of PBGFs have been investigated, including solid-core PBGFs and hollow-core PBGFs. The validation of the approximate theoretical model has been proved by numerical results. According to the ARROW model and numerical results, the cut-offs of all modes in individual high-index inclusions are responsible for the formation of stop bands. However, their widths become increasingly narrow with the increment of the order of the modes. For hollow-core PBGFs, the wavelength shifts of the locations of bandgaps can be estimated by using refractive index scaling law, which is derived by using scalar wave approximation. Therefore, the refractive index scaling law is strictly valid for the hollow-core PBGFs with large air-filling fraction and small index contrast. Both ARROW model and refractive index scaling law provide simple analytical tools for designing PBGFs based

biochemical sensors. In addition, these two models are not limited in the isotropic situation. They can be extended to anisotropic PBGFs and facilitate the analysis and design of anisotropic PBGFs based biochemical sensors.

Chapter 4

Anisotropic Photonic Bandgap Fibers

4.1 Introduction

Most of the research efforts aim to theoretically simulate and experimentally demonstrate the isotropic photonic bandgap fibers (PBGFs) based biochemical sensors. However, several novel applications of liquid crystal (LC) biosensors have been demonstrate recently and attract a lot of research attention. The perspectives of design and active control of PCFs are further widened, if the idea of self-organised material components is brought into action, such as LCs, which may be used in three-dimensional photonic crystals to obtain tunable light localization, or to allow mirrorless lasing through the formation of a self-assembled photonic bandgap (PBG) material [84, 128]. It is, therefore, fundamentally interesting to study the potential application of LCs as means of introducing enhanced periodicity and controllability, and in a further sense make the two-dimensional PCF a three-dimensional structure. Combining this with the knowledge of LCs in biological system, such as DNA and cell membranes, could open up for a new class of photonic bandgap fiber (PBGF) based biosensors with sub-microliter sample volume [47-49]. Further, it has been shown that LCs could act as an optical amplifier of

protein-ligand bindings, which further strengthens the possibility of using LCs infiltrated PCFs as biosensors for detection of receptor binding of certain molecules, e.g., proteins [47, 48, 129]. However, the complex structure of LCs infiltrated PBGFs, in particular, the anisotropic nature of LCs, makes its electromagnetic analysis challenging [130, 131]. Driving by all these advantages of LCs infiltrated PCFs based biosensing devices, the theoretical and numerical modeling are thus of practical importance for nanophotonics and biomedical research.

In this chapter, the theoretical and numerical models of anisotropic PBGFs are presented. One of the most common LC phases is the nematic, where the molecules have no positional order, but they have long-range orientational order. Thus, the molecules flow and their center of mass positions are randomly distributed as in a liquid, but they all point in the same direction (within each domain). Most nematics are uniaxial: they have one axis that is longer and preferred, with the other two being equivalent (can be approximated as cylinders). The emphasis therefore has been put on the investigation on the shifts of the transmission windows or bandgaps with the variation of ordinary and extraordinary refractive index of nematic LCs (NLCs), which is discussed in Section 4.2. The effect of the orientation of NLCs on the bandgap formation has also been investigated, which is demonstrated in Section 4.3. Similarly, the anisotropic PBGFs are grouped according to core and cladding composition. Based on the selection of the background material and provided that $n_e > n_o$, three possible configurations of the PBGFs are found with $n_b < n_o < n_e$, $n_e > n_b > n_o$ and $n_b > n_e > n_o$, where n_b , n_e and n_o are background

refractive index, extraordinary and ordinary refractive indices of NLCs, respectively. These conditions can be satisfied by the selection of nonsilica glasses as background material, including chalcogenide glasses, tellurite glasses, and other heavy metal oxide glasses which have a typical refractive index range from 1.5 to 2.5 [132-134]. The corresponding features of the bandgaps are discussed in Sections 4.4, 4.4.2 and 4.5, respectively. It is worthy noting that the developed analytical models are general, which can also be applied to investigate the bandgap shifts due to thermo-tuning or electrical tuning.

4.2 Refractive index scaling law for anisotropic PBGFs

Fig. 4.1(a) and (b) shows an all silica solid-core PBGF with NLC inclusions and a high-index hollow-core PBGF with NLC inclusions, respectively. Following the previous designation, the diameters and spacing of the cylindrical NLC inclusions are d and Λ , respectively. The dielectric tensors of the background material and NLC inclusions are $\epsilon_b = n_b^2$ and ϵ_a , respectively. For the all silica solid-core PBGF, n_b is assumed to be smaller than both n_o and n_e . On the other hand, for the high-index hollow core PBGF, n_b is assumed to be larger than both n_o and n_e . In particular, the extraordinary axis is assumed to lie along the fiber axis (z -direction). Consequently, ϵ_a takes the forms of $\epsilon_a = \text{diag}(n_o^2, n_o^2, n_e^2)$. This alignment can theoretically be exhibited under the influence of the appropriate homeotropic anchoring conditions [84]. It should be noted that the discussion is focused on the tuning of transmission windows, which relies on the scaling of the

extraordinary and ordinary indices of the NLCs. The wavelength shifts of the transmission windows due to the orientation of the NLCs are not considered here and will be discussed in Section 4.3. The wavelength- and temperature-dependent refractive indices of NLC compounds and mixtures can be described by the extended Cauchy equations as explicit functions [135]. In the following, $n_o(\lambda, T)$ and $n_e(\lambda, T)$ are simply written as n_o and n_e for the sake of discussion.

Fig. 4.1: (a) All silica solid-core PBGF with NLC inclusions, (b) high-index hollow-core PBGF with NLC inclusions.

The corresponding dielectric tensor of photonic crystal (PC) claddings can thus be described as $\epsilon(x,y)=\text{diag}(n_{xx}^2(x,y), n_{yy}^2(x,y), n_{zz}^2(x,y))$, where $n_{xx}=n_{yy}\neq n_{zz}$. A pair of coupled equations for $E_x(x, y)$ and $E_y(x, y)$, which are the polarization components of $\mathbf{E}$ along the x and the y directions, can be derived as [95]

$$\begin{aligned} \frac{\partial^2 E_x}{\partial y^2} + \frac{\partial}{\partial x} \left[\frac{1}{n_{zz}^2} \frac{\partial}{\partial x} (n_{xx}^2 E_x) \right] + (n_{xx}^2 k_0^2 - \beta^2) E_x \\ = \frac{\partial^2 E_y}{\partial x \partial y} - \frac{\partial}{\partial x} \left[\frac{1}{n_{zz}^2} \frac{\partial}{\partial y} (n_{yy}^2 E_y) \right] \end{aligned} \quad (4.1)$$

$$\begin{aligned} \frac{\partial^2 E_y}{\partial x^2} + \frac{\partial}{\partial y} \left[\frac{1}{n_{zz}^2} \frac{\partial}{\partial y} (n_{yy}^2 E_y) \right] + (n_{yy}^2 k_0^2 - \beta^2) E_y \\ = \frac{\partial^2 E_x}{\partial x \partial y} - \frac{\partial}{\partial y} \left[\frac{1}{n_{zz}^2} \frac{\partial}{\partial x} (n_{xx}^2 E_x) \right] \end{aligned} \quad (4.2)$$

where k_0 is a free-space wave constant with the value of $2\pi/\lambda$, β is a propagation constant.

Analogous to its isotropic counterpart, the polarization and coupling dependence of the propagating waves can be ignored, assuming small refractive index contrast and low anisotropy. This approximate scalar method has been extensively used in the analysis of three-dimensional anisotropic optical waveguides [114, 115, 136]. The validity of this approach has been demonstrated by analyzing the optical waveguides with large anisotropy, such as $n_0=2.25$ and $n_e=2.172$ [115] and anisotropic optical waveguide having a permittivity tensor with nonzero off-diagonal elements [114, 115, 136]. In order to derive the refractive index scaling law, scalar wave approximation is extended to the analysis of anisotropic photonic bandgap fiber.

The scalar approximation yields a pair of decoupled scalar equations, which are given by

$$\frac{\partial^2 E_x}{\partial y^2} + \frac{n_{xx}^2}{n_{zz}^2} \frac{\partial^2 E_x}{\partial x^2} + (n_{xx}^2 k_0^2 - \beta^2) E_x = 0 \quad (4.3)$$

$$\frac{\partial^2 E_y}{\partial x^2} + \frac{n_{xx}^2}{n_{zz}^2} \frac{\partial^2 E_y}{\partial y^2} + (n_{xx}^2 k_0^2 - \beta^2) E_y = 0 \quad (4.4)$$

The polarization coupling items on the right-hand side of Eqs. (4.1) and (4.2) are ignored, as they have negligible effect on the bandgap formation [130]. When observing Eqs.(4.3) and (4.4), it is found that they are of no difference except for the exchanged x - and y -axis. Therefore, only one of the equations in Eqs.(4.3) and (4.4) is enough to evaluate the bandgaps of the anisotropic dielectric structure. Consequently, the refractive index scaling law can be obtained by analyzing only one of the equations. Taking the example of Eq.(4.3), it can be re-cast in terms of normalized transverse coordinates $X=x/\Lambda$ and $Y=y/\Lambda$ and an index distribution function

$$g(X,Y) = \begin{cases} 0 & \text{low index regions} \\ 1 & \text{high index regions} \end{cases} \quad (4.5)$$

and the resulting normalized scalar wave equation is

$$\frac{\partial^2 E_x}{\partial Y^2} + \frac{\partial^2 E_x}{\partial X^2} + h(X,Y) \cdot \left(\frac{n_o}{n_e} - 1 \right) \cdot \frac{\partial^2 E_x}{\partial X^2} + (v^2 f(X,Y) - w^2) E_x = 0 \quad (4.6)$$

where $h(X,Y) = g(X,Y)$, $v^2 = \Lambda^2 k^2 (n_o^2 - n_b^2)$ and $w^2 = \Lambda^2 (\beta^2 - k^2 n_b^2)$ for Fig. 4.1(a) and $h(X,Y) = (1 - g(X,Y))$, $v^2 = \Lambda^2 k^2 (n_b^2 - n_o^2)$ and $w^2 = \Lambda^2 (\beta^2 - k^2 n_o^2)$ for Fig. 4.1(b).

The difference between the scalar wave equations for anisotropic and isotropic dielectric structures is obvious. In the differential operator, an extra term is found, which comprises the information of anisotropy. Supposing that the dielectric structure is isotropic with $n_o = n_e$, this additional term vanishes, which leads to a familiar scalar wave

equation for isotropic dielectric structures. Therefore, a similar refractive index scaling law can be described as the following. From Eq.(4.6), the eigenvalues w^2 of its modes E_x are determined by v^2 , $g(x, y)$ and n_o/n_e . Given a fixed value of the ratio n_o/n_e , if k , Λ , n_o or n_b vary, the photonic states scale so that v^2 and w^2 are invariant.

The refractive index scaling law enables the study of photonic states on either side of the “core line” in a continuous manner. The core line represents $n_{eff}=n_b$ for Fig. 4.1(a) and $n_{eff}=n_o$ for Fig. 4.1(b), respectively. More in particular, when examining the invariant v , the normalized operating wavelength λ/Λ of the bandgaps is found to be proportional to the refractive index contrast $\sqrt{|n_b^2 - n_o^2|}$, which can be given by

$$\lambda/\Lambda = C \sqrt{|n_b^2 - n_o^2|} \quad (4.7)$$

where C is a constant.

Before applying the refractive index scaling law including Eq.(4.7), a precondition is needed to be met which requires the ratio n_o/n_e is invariant during the scaling process. For example, during the thermo-tuning process, in order to apply the refractive index scaling law to evaluate its performance, the ratio n_o/n_e should be independent of temperature. This is impractical. However, if the ratio n_o/n_e plays a minor role in determining the refractive index scaling, the precondition could be neglected, which gives an approximate refractive index scaling law but greatly simplifies the analysis process. This will be investigated in the following Section 4.2.1.

4.2.1 All silica solid-core PBGF with NLC inclusions

In the following, the bandgaps in the anisotropic PC cladding are evaluated by using the full-vector plane-wave expansion method [137]. The NLC is assumed to be E7, which has an ordinary and extraordinary refractive index $n_o=1.52$ and $n_e=1.75$, respectively [84]. The parameters are defined as $n_b=1.45$ and $d=0.4\Lambda$, respectively.

Fig. 4.2 represents the gap map of an all silica solid-core PBGF with NLC inclusions. It is relatively easy to analyze the bandgaps of all silica solid-core PBGF with NLC inclusions. It has been shown recently that the band structure of low-contrast PBGFs could be predicted from the modal analysis of individual high-index inclusions, according to the antiresonant reflecting optical waveguide (ARROW) model [116, 131]. In particular, photonic bandgap edges (PBEs) can be evaluated by examining the modal cutoffs. The modal cutoffs for the uniaxial fibers have close-form analytical solutions, which are described as [70, 131]

$m = 0$	$J_0(U) = 0 \quad (\text{TE}_{0l} \text{ mode})$	$J_0(\kappa_{co}U) = 0 \quad (\text{TM}_{0l} \text{ mode})$
$m = 1$	$J_1(U) = 0 \quad (\text{HE}_{1l} \text{ mode})$	$J_1(\kappa_{co}U) = 0 \quad (\text{EH}_{1l} \text{ mode})$
$m \geq 2$	$J_{m-1}(U)J_m(\kappa_{co}U) + \kappa_{co} \left(n_o/n_b\right)^2 J_m(U)J_{m-1}(\kappa_{co}U) - U/(m-1) J_m(U)J_m(\kappa_{co}U) = 0$	

Table 4-1: Modal cutoffs of a step-profile uniaxial fiber with an anisotropic core and an isotropic cladding.

The analytical solutions show good agreement with the simulation results, which are demonstrated as the vertical arrows. More in particular, it is clear from Table 4-1 that

the locations of the bandgaps are determined by the ratio n_o/n_e and $\sqrt{n_o^2 - n_b^2}$, which agrees well with the refractive index scaling law.

Fig. 4.2: Gap map of the PC cladding in with $\varepsilon_a = \text{diag}(n_o^2, n_o^2, n_e^2)$. Arrows indicate the modal cutoffs of an individual cylindrical rod with $\varepsilon_a = \text{diag}(n_o^2, n_o^2, n_e^2)$.

4.2.2 High-index hollow-core PCF with NLC inclusions

The parameters used here are defined as $n_b=2$, $n_o=1.52$, $n_e=1.75$ and $d=0.9\Lambda$, respectively. These conditions can be satisfied by the selection of nonsilica glasses as background material, including chalcogenide glasses, tellurite glasses, and other heavy metal oxide glasses, which have a typical refractive index range from 1.5 to 2.5 [25, 138].

Fig. 4.3: Gap maps of the PC claddings with $\epsilon_a = \text{diag}(n_o^2, n_o^2, n_e^2)$ and $\epsilon_a = n_o^2$.

Similar to the isotropic hollow-core PBGFs, it is also unfeasible to obtain explicit expressions for model cutoffs of the anisotropic hollow-core PBGFs. In order to understand the anisotropic effect on the bandgap formation, a comparison between the bandgaps of anisotropic PBGFs and isotropic PBGFs is required. Fig. 4.3 represents the gap map of the PC claddings with $\epsilon_a = \text{diag}(n_o^2, n_o^2, n_e^2)$ and $\epsilon_a = n_o^2$, respectively. It is found that the presence of material anisotropy renders a similar bandgap structure as the isotropic PBGF, which is different from the comparison between isotropic and anisotropic solid-core PBGFs. In order to explain this distinct behavior, it is necessary to examine the PC cladding as shown in Fig. 4.1(b). Taking the assumption that bridges are thin enough, the whole structure can be described as approximately cylindrical nonsilica rods embedded in the anisotropic NLCs as shown in Fig. 4.4 [139]. The band structure of low contrast bandgap fibers in Fig. 4.4 could be predicted from the modal analysis of

individual high-index inclusions, according to the ARROW model. However, unlike the fiber structure shown in Fig. 4.1(a), an individual high-index inclusion in Fig. 4.4 has an isotropic core and anisotropic claddings. Therefore, the modal cutoffs also differ from those shown in Table 4-1. Close-form analytical solutions exist for the modal cutoffs of the cylindrical waveguides with anisotropic cladding, which are described as [70, 131]

m = 0	$J_0(U) = 0$ (TE _{0l} and TM _{0l} modes)
m = 1	$J_1(U) = 0$ (HE _{1l} and EH _{1l} modes)
m ≥ 2	$\left(1 + (n_b/n_o)^2\right) J_m(U) J_{m-1}(U) - U(1 + \kappa_{cl}^2) / (2(m-1)) J_m^2(U) = 0$

Table 4-2: Modal cutoffs of a step-profile uniaxial fiber with an isotropic core and an anisotropic cladding.

As clear from Table 4-2, the modal cutoffs of TE_{0l}, TM_{0l}, HE_{1l} and EH_{1l} (*l*=1, 2, 3...) modes for these cylindrical waveguides with anisotropic cladding are exactly the same as the isotropic case. This certainly yields a similar band structure. The deviation from the isotropic counterpart might be the results of irregular shape of nonsilica block and the interactions of these nonsilica blocks linked by the bridges.

Fig. 4.4: Ideal anisotropic PBGF derived from Fig. 4.1(b).

This similarity raises a question of whether the extraordinary index of NLC along the fiber axis has a negligible effect on the bandgap formation. To answer this question, the shifts of the PBG-guiding wavelength ranges, which are the spans where the core line $n_{eff}=n_o$ crosses the gap region, have been plotted versus the extraordinary index of NLC in Fig. 4.5. In the simulation, ordinary index n_o was kept fixed as 1.52, whereas extraordinary index n_e was varied from 1.2 to 1.9. It is observed that excepting the secondary PBG, the operating wavelengths of the PBGs have a red-shift, along with an increment in the wavelength spans. On the contrary, the wavelength span of the secondary bandgap shrinks with the increment of extraordinary index n_e and finally closes up. The contrary behaviors might be interpreted as their difference in the bandgap formation. As shown later, the secondary bandgap is formed by the vector effects, whereas the others are mainly formed by scalar effects. Analyzing these behaviors is not

straightforward from Eq.(4.6), since there is an index distribution function appearing in the differential operator. However, when examining Fig. 4.5, it is found that although the extraordinary index n_e has a large variation ranging from 1.2 to 1.9, the PBG-guiding wavelength ranges shift slightly, especially for the higher order bandgaps. The results further confirm the previous analysis. Although the ratio n_o/n_e cannot remain fixed during the temperature change, for example, the extraordinary index plays a minor role in determining the shifts of bandgaps. Therefore, by ignoring the anisotropic effect, a simple equation of Eq.(4.7) can describe the refractive index scaling law approximately.

Fig. 4.5: PBG-guiding wavelength ranges as a function of n_e .

In order to demonstrate the validity of Eq.(4.7), Fig. 4.6 shows the PBG-guiding wavelength ranges as a function of the refractive index contrast $\sqrt{n_b^2 - n_o^2}$. In the simulation, ordinary index n_o varies from 1.3 to 1.995, whereas extraordinary index n_e

was kept fixed as 1.75. For most of the bandgaps in Fig. 4.6, the normalized operating wavelength λ/Λ of the bandgaps is simply proportional to the refractive index contrast, which certainly corresponds to the analysis, especially when the refractive index contrast is small. It further confirms that the anisotropy effect plays a minor role on the wavelength shifts of the PBGs. Moreover, although the wavelength spans keep increased in the beginning, they start to reduce in size when the refractive index contrast is large enough. This could be appreciated by considering the vector effects. General speaking, the overall bandgap can be constructed by the overlap of the bandgaps of two orthogonal polarization components. When the refractive index contrast is small, these two polarization components are degenerated and their bandgaps are completely overlapped, which could be seen from Eqs.(4.3) and (4.4). However, as the refractive index contrast increases, these two polarization components become split and the overlap region of bandgaps becomes narrower. Although most of the bandgaps open up at very small refractive index contrast, exceptions are also found, which appear and open up for a large refractive index contrast. This could be the result of vector effect, which comes into effect when the refractive index contrast is large enough [126, 140]. In addition, the wavelength spans of these bandgaps become narrower and completely close up as the refractive index contrast increases. One of the reasons that bring about this feature is the material anisotropy. When the refractive index contrast increases, the ratio n_e/n_o becomes larger. As seen from the secondary bandgap in Fig. 4.5, this gives rise to reduced wavelength spans of PBGs formed by vector effect. Consequently, the wavelength spans

of the secondary bandgap have an increase for the small refractive index contrast followed by a reduction when the refractive index contrast becomes large.

Fig. 4.6: PBG-guiding wavelength ranges as a function of $\sqrt{n_b^2 - n_o^2}$.

Although the refractive index scaling law is strictly valid for small refractive index contrast, it shows a good agreement with the simulation results and correctly locates the specific features in the band structures. This greatly facilitates the investigation of tuning of transmission windows due to the scaling of the extraordinary and ordinary indices. According to the extended Cauchy equations, the temperature effect can be simply incorporated into the extraordinary and ordinary refractive indices n_e and n_o of the NLCs to study the wavelength shifts of the transmission windows.

4.3 Effect of liquid crystal alignment on bandgap formation

Fig. 4.7: (a) Cross section of the anisotropic PBGF. (b) NLC with optic axis along z direction. (c) NLC with optic axis along y direction.

The anisotropic feature of NLC introduces a unique tuning method of bandgaps through the orientation of NLCs. Fig. 4.7(a) shows an anisotropic PBGF made of high-index anisotropic NLC rods with dielectric tensor of ϵ_a immersed in low-index silica background with dielectric tensor of ϵ_b . Two specific alignments of the NLC are demonstrated in Fig. 4.7(b) and (c). Following the designations, the PC cladding can be characterized by two parameters: hole-to-hole distance Λ , hole size d . NLC has a rod-like structure with an ordinary refractive index of n_o and an extraordinary refractive index of n_e , respectively. Therefore, it is expected that different alignments of NLC can change the

dielectric tensor ε_a . For example, the dielectric tensor ε_a take the forms of $\varepsilon_a = \text{diag}(n_o^2, n_o^2, n_e^2)$ and $\varepsilon_a = \text{diag}(n_o^2, n_e^2, n_o^2)$ for the alignments shown in Fig. 4.7(b) and Fig. 4.7(c), respectively. Both alignments can be theoretically exhibited under the influence of the appropriate homeotropic anchoring conditions or by the application of an external electric (or magnetic) static field across the fiber [84]. The corresponding dielectric tensor of PC claddings can thus be described as $\varepsilon(x,y) = \text{diag}(n_{xx}^2(x,y), n_{yy}^2(x,y), n_{zz}^2(x,y))$. In order to characterize the bandgaps in the PC cladding, a pair of coupled equations for $E_x(x, y)$ and $E_y(x, y)$, which are the polarization components of $\mathbf{E}$ along x and y directions, can be derived

The coupling terms are ignored by assuming small refractive index contrast and low anisotropy, which simplifies the analysis. In particular, when $\varepsilon_a = \text{diag}(n_o^2, n_o^2, n_e^2)$ or $n_{xx} = n_{yy} \neq n_{zz}$, ignoring the coupling terms leads to a pair of decoupled equations for E_x and E_y , which is given by

$$\frac{\partial^2 E_x}{\partial y^2} + \frac{\partial}{\partial x} \left[\frac{1}{n_{zz}^2} \frac{\partial}{\partial x} (n_{xx}^2 E_x) \right] + (n_{xx}^2 k_0^2 - \beta^2) E_x = 0 \quad (4.8)$$

$$\frac{\partial^2 E_y}{\partial x^2} + \frac{\partial}{\partial y} \left[\frac{1}{n_{zz}^2} \frac{\partial}{\partial y} (n_{xx}^2 E_y) \right] + (n_{xx}^2 k_0^2 - \beta^2) E_y = 0 \quad (4.9)$$

Eqs. (4.8) and (4.9) are of no difference, excepting the exchanged x and y axis. Therefore, there is also no difference between the corresponding bandgaps for E_x and E_y . In other words, only one of Eqs. (4.8) and (4.9) is necessary to evaluate the full band structure.

When $\varepsilon_a = \text{diag}(n_o^2, n_e^2, n_o^2)$ or $n_{xx} = n_{zz} \neq n_{yy}$, ignoring the coupling terms gives rise to

$$\frac{\partial^2 E_x}{\partial y^2} + \frac{\partial}{\partial x} \left[\frac{1}{n_{xx}^2} \frac{\partial}{\partial x} (n_{xx}^2 E_x) \right] + (n_{xx}^2 k_0^2 - \beta^2) E_x = 0 \quad (4.10)$$

$$\frac{\partial^2 E_y}{\partial x^2} + \frac{\partial}{\partial y} \left[\frac{1}{n_{yy}^2} \frac{\partial}{\partial y} (n_{yy}^2 E_y) \right] + (n_{yy}^2 k_0^2 - \beta^2) E_y = 0 \quad (4.11)$$

A direct comparison of Eqs. (4.10) with (4.11) illustrates the alignment effect on the bandgap formation. Band structure of E_x can be evaluated by using the PC cladding with $\varepsilon_a = n_o^2$; whereas, the band structure of E_y can be evaluated by using the PC cladding with $\varepsilon_a = \text{diag}(n_e^2, n_e^2, n_o^2)$. The absolute gap regions are simply the overlap regions of the bandgaps of E_x and E_y .

Fig. 4.2 represents the gap map for the PC cladding containing NLC oriented along z direction, where $\varepsilon_a = \text{diag}(n_o^2, n_o^2, n_e^2)$. The PBG-guiding wavelength ranges in a silica core can be easily identified, which are the spans where the core line $n_{eff} = 1.45$ crosses the gap regions. It has been shown recently that the band structure of low contrast bandgap fibers could be predicted from the modal analysis of individual high-index inclusions, according to the ARROW model [118, 122, 131]. Particularly, PBEs can be evaluated by examining the modal cut-offs. Close-form analytical solutions exist for the modal cut-offs of the step-index uniaxial fiber, which show good agreement with the simulation results as demonstrated as vertical arrows.

The orientation of the optic axis along y direction leads to a change in the bandgaps. The gap map obtained with a full-vectorial model is demonstrated in Fig. 4.8(a), whereas Fig. 4.8(b) was obtained by the approximation ignoring the coupling effect according to

Eqs. (4.10) and (4.11). By comparing Fig. 4.8 (a) with Fig. 4.8(b), it is easy to identify some practically interesting guiding regions. Above the radiation line of E_y , it is a region where index-guiding is able to be achieved for both E_x and E_y . Between the two radiation lines, the guidance mechanisms for the two polarization components are different: E_x is guided by index-guiding effect, whereas E_y is guided by bandgap effect. Under the radiation line of E_x , both E_x and E_y exhibit the behavior of bandgap guidance and the absolute gap structure is determined by the overlap of the gap regions. Modal analysis of transversely anisotropic cylinder waveguides requires tedious numerical work, as close-form analytical solutions do not exist. However, as seen from Eqs. (4.10) and (4.11), the locations of the PBEs can alternatively be estimated by evaluating the PBEs of E_x and E_y , which has explicit expressions. A good agreement is found between the analytical results and simulation results.

This simple approximation renders surprisingly good qualitative results despite the high anisotropy of the cylindrical rods. A qualitative understanding can be performed by examining the coupling terms in Eqs.(4.10) and (4.11), which are the only term neglected in the derivation. Two parameters determine the coupling terms, including the index contrast n_o/n_b and n_e/n_b and anisotropy n_e/n_o . It has been found in the isotropic case, that the coupling terms cannot be neglected only when the index contrast is significantly large [126]. Similarly, for the anisotropic case, the coupling terms come into effect when index contrast and/or anisotropy cannot be ignored, which requires $n_o/n_b \gg 1$, $n_e/n_b \gg 1$ and/or

$n_e/n_o \gg 1$. For a large range of NLC, these conditions cannot be satisfied. Therefore, ignoring coupling terms yields little change to the bandgaps.

Fig. 4.8: (a) Gap map of the PC cladding with $\epsilon_a = \text{diag}(n_o^2, n_e^2, n_o^2)$ by using full-vectorial model and (b) by using the approximation which ignores the coupling effect. Arrows indicate the modal cutoffs of an individual cylindrical rod with $\epsilon_a = n_o^2$ and $\epsilon_a = \text{diag}(n_e^2, n_e^2, n_o^2)$, respectively.

The modal dispersion curves of fundamental modes as a function of the normalized wavelength are shown in Fig. 4.9, which were obtained by using a full-vectorial BPM [95]. As indicated by Eqs. (4.10) and (4.11), the anisotropy splits the propagation constants of E_x and E_y , which can be observed inside the overlap bandgaps of E_x and E_y and in the wavelength range from 0.55 to 0.62, where a high birefringence in an order of 10^{-2} can be achieved. In the rest of the bandgaps, only single-polarized modes exist. The field distributions of the fundamental modes in the inset figures show a good agreement with the ARROW model. At the wavelengths inside their respective bandgaps, the fundamental modes of E_x and E_y are spatially confined within the silica core with similar field distributions. Outside their respective bandgaps, the resonance occurs inside the high-index cylindrical rods.

Fig. 4.9: Modal dispersion curves of fundamental modes as a function of the wavelength. Inset figures: field distributions of E_x and E_y .

4.4 Solid-core anisotropic PBGFs

4.4.1 Photonic Bandgap Guiding ($n_b < n_e$ and $n_b < n_o$)

The dielectric structure of solid-core anisotropic PBGFs are demonstrated in Fig. 4.1(a) with NLC inclusions and optics axis is assumed to be along z direction. As previously described, the band structure of low contrast isotropic bandgap fibers could be predicted from the modal analysis of individual high-index inclusions, according to the ARROW model. However, there are at least two important issues that need to be settled. First, it is necessary to understand which mode in the NLC infiltrated cylindrical rods leads to the appearance of the transmission dips of the entire structure. For the isotropic case, it has been found that the stop bands become increasingly narrow with the increment of orders. Therefore, it may also conclude that only specific resonant conditions in the NLC infiltrated cylindrical rods can result in the transmission dips. Secondly, obtaining explicit expressions for the modal cutoffs of those specific modes is crucial for simplifying both design and analysis procedure.

The resonant conditions in a uniaxial cylindrical waveguide are well understood [70]. The electromagnetic wave equations that govern the propagation characteristics of guided optical modes can be decoupled if z is the wave propagation direction and also the fiber axis. More in particular, the modal cutoffs have close-form analytical solution. Given an isotropic material with $n_e = n_o$, the modal cutoffs of TE_{0l} and TM_{0l} as well as

HE_{1l} and EH_{1l} are degenerate. As the locations of transmission minima are related to the modal cutoffs, the anisotropy may lead to more transmission dips due to the split of the degeneracy of the modal cutoffs.

Fig. 4.10 shows the transmission spectra for an isotropic PBGF and an anisotropic PBGF, respectively, which provide a visual understanding of the effects of material anisotropy. The parameters are chosen as follows: $d=1.55\mu\text{m}$, $\Lambda=5\mu\text{m}$, $n_b=1.45$, $n_e=1.7$ and $n_o=1.5$. The selection of $n_e=1.7$ and $n_o=1.5$ is for the reason that most NLCs have n_e around 1.7 and n_o around 1.5, especially in the long wavelengths [84]. In isotropic case, it is assumed that $n_e=n_o$. The transmission spectra were evaluated by using a full-vectorial beam propagation method and taken after beam propagated along the fiber (in z direction) at $z=1\text{mm}$. Three layers were used in the simulations. Clearly, the number of transmission dips for the anisotropic case is doubled compared to the isotropic counterpart. In particular, a number of transmission dips for the anisotropic case exhibits spectral overlap with those for the isotropic counterpart. Besides, additional transmission dips for anisotropic case are found, which are believed to be the results of the split of the degeneracy of the modal cutoffs. This can be clarified by examining the field distribution of the propagation modes at the wavelength corresponding to the transmission minima. Fig. 4.11(i(a)) and (ii(a)) shows the mode intensity and electric vector distributions inside the high-index inclusions at $0.787\mu\text{m}$ for the isotropic structure. Complying with the ARROW model, the resonance occurs inside the high-index cylindrical rods at transmission minima. Moreover, the electric field inside the high-index inclusion is

nearly linear polarized, which arise from the modal degeneracy. This degeneracy can be lifted by the introduction of anisotropy, which brings in additional transmission dips. Fig. 4.11(i(b)) and (ii(b)) shows the mode intensity and electric vector distributions inside the high-index inclusions at $0.787\mu\text{m}$ for the anisotropic structure. Similarly, the mode intensity and electric vector distributions at $0.886\mu\text{m}$ are demonstrated in Fig. 4.11(i(c)) and (ii(c)), respectively. It is thus clear that the anisotropy leads to a resonance of TE_{01} and TM_{01} modes inside the NLC inclusion at the wavelength of $0.787\mu\text{m}$ and $0.886\mu\text{m}$, respectively. In order to illustrate this idea, the resonance conditions at the wavelength corresponding to the transmission minima are all labeled in Fig. 4.10.

Fig. 4.10: Transmission spectra for an isotropic PBGF and an anisotropic PBGF. The analytical cutoff wavelengths are marked as vertical arrows.

Fig. 4.11: Modal intensity distribution and electric vector distribution for (a) isotropic PBGF at $0.787\mu\text{m}$, anisotropic PBGF (b) at $0.787\mu\text{m}$ and (c) $0.886\mu\text{m}$.

Clearly from Fig. 4.10, it is found that the modal cutoffs of TM_{0l} , TE_{0l} , HE_{1l} , EH_{1l} , HE_{2l} and EH_{2l} modes contribute to the appearance of transmission dips. It has been shown that the loss of each transmission minima is dependent on an important parameter of an optical fiber, which is the fraction of power residing in the core η [124]. In particular, the modal group velocity of the modes with $\eta=0$ at cutoff approaches the speed of light in the cladding. This leads to the effective index of the cylindrical rods equal to that of the silica background and thus yields high loss. In fact, the mode with $\eta>0$ at cutoff could also lead a transmission dip, but the corresponding amplitude depends on the value of η . For the modes with $\eta\approx 0$, the corresponding transmission minima are expected

to be significantly deep. However, for the modes with $\eta \gg 0$, the amplitudes of corresponding transmission minima are extremely small. It has been demonstrated that the property of η in a uniaxial fiber is analogous to its isotropic counterpart [141]. Therefore, TE_{0l} , TM_{0l} , HE_{1l} and HE_{2l} modes are found with $\eta=0$ at cutoffs, which are followed by EH_{1l} , EH_{2l} and HE_{3l} modes with η closest to 0. The reason that HE_{3l} mode do not manifest in the transmission spectrum is simply for the reason that its modal cutoff coincides with HE_{12} mode, which has $\eta=0$. In other words, the amplitude of the corresponding transmission dip is relatively small compared to that formed by HE_{12} mode. As a result, only TM_{0l} , TE_{0l} , HE_{1l} , EH_{1l} , HE_{2l} and EH_{2l} modes are responsible for the high loss transmission dips.

Fig. 4.12: Transmission spectra for the solid-core anisotropic PBGF with different pitches.

Fig. 4.12 shows the transmission spectra for the solid-core anisotropic PBGF with different Λ while d is invariant as $1.55\mu\text{m}$, which make it easy to understand the effect of η . It has been demonstrated increasing Λ yields lower loss, provided d is invariant. A qualitative understanding of this behavior can be appreciated by considering the size of the core, which has a diameter of 2Λ . Increasing Λ effectively enlarges the core, which thus enhance the confinement of the core and leads to lower loss. On the contrary, when Λ changes from $5\mu\text{m}$ to $2.5\mu\text{m}$, the confinement of the light should become weak and hence even the modes with $\eta \gg 0$ could lead to the appearances of more transmission dips. This certainly complies with the observation from Fig. 4.12. Moreover, the locations of the transmission dips are barely altered, as d is kept invariant. An alternative way to modify the loss property is adjusting the number of rings [118-120]. Fig. 4.13 demonstrates the transmission spectra for the solid-core anisotropic PBGF with different number of rings. Increasing the number of rings greatly reduces the loss of transmission dips, which agrees well with the isotropic case. As a result, only the transmission dips which are derived by the modes with η equal to or closest to 0 could survive and manifest in the transmission spectrum. Since the commercialized PCF usually have six or more rings, only the locations of transmission dips derived from TM_{0l} , TE_{0l} , HE_{1l} , EH_{1l} , HE_{2l} and EH_{2l} modes are considered necessary.

Fig. 4.13: Transmission spectra for the solid-core anisotropic PBGF with different number of rings.

Therefore, in order to predict the locations of these transmission dips, it is necessary to obtain the modal cutoff wavelengths for the TM_{0l} , TE_{0l} , HE_{1l} , EH_{1l} , HE_{2l} and EH_{2l} modes. The exact solution of the cutoff wavelengths of these modes with respect to κ_{co} ($\kappa_{co} = n_e/n_o$) are shown in Fig. 4.14. Based on Fig. 4.14, it can be concluded that only the locations of the transmission dips which are derived from TM_{0l} , EH_{1l} and EH_{2l} shift when the anisotropy of the infiltrated NLC varies. In addition, the cutoff wavelengths of the HE_{2l} and EH_{2l} nearly coincide with the cutoff wavelengths of the TE_{0l} and TM_{0l} modes, respectively.

Fig. 4.14: Exact solution of the cutoff wavelengths vs. κ_{co} .

Explicit expressions can be found for the modal cutoffs by using cosine approximation for the Bessel function $J_v(U)$, when $U \gg v$. The locations of the transmission dips which are derived from TE_{0l} , HE_{1l} and HE_{2l} modes can be described as

$$\lambda_m = \frac{2d\sqrt{n_o^2 - n_b^2}}{m + 1/2} \quad m=1, 2, \dots \quad (4.12)$$

where m is the order of the transmission dips and counted from longer wavelength side. Eq.(4.12) is identical to the isotropic case, which thus renders the overlap transmission dips in Fig. 4.10.

According to the equations in Table 4-1, the locations of the transmission dips which are derived from TM_{0l} , EH_{1m} and EH_{2m} modes can be simply described as

$$\lambda_{m'} = \frac{n_e}{n_o} \cdot \frac{2d\sqrt{n_o^2 - n_b^2}}{m' + 1/2} \quad m'=1, 2, \dots \quad (4.13)$$

where m' is the order of the transmission dips and counted from longer wavelength side.

The validity of the cosine approximation is able to be evaluated by compare the exact solution and cosine approximation. Fig. 4.15 shows the locations of the transmission dips by using exact solution and cosine approximation, respectively. It is worthy noting that the absolute wavelength errors caused by the cosine approximation greatly decreases with the increment of the order m or m' . In particular, when m or $m' > 4$, the estimated errors are less than $10^{-3} \mu\text{m}$. Therefore, the cosine approximation provides simple tools for analyzing the locations of the transmission dips.

Fig. 4.15: Comparison of exact solution and cosine approximation of modal cutoffs.

4.4.2 Hybrid guiding ($n_o < n_b < n_e$)

The structure of the hybrid guiding anisotropic PCF is demonstrated in Fig. 4.1(a). The refractive index of the background material is assumed to be n_b and has the value of $n_e > n_b > n_o$. The optic axis of NLC is considered to be uniform and parallel to the y-axis of

the fiber's lattice. Consequently, the dielectric tensor of the NLC inclusions takes the form of $\epsilon_a = \text{diag}(n_o^2, n_e^2, n_o^2)$. The guiding mechanisms for the two polarization components are affected by this selection of background material. By intuition, light of the x polarization senses a PCF with the refractive index of the core larger than that of the cladding and thus can be considered to be guided by total internal reflection (TIR). On the other hand, the y -polarized light senses a PCF with the refractive index of the core smaller than that of the cladding, which corresponds to PBG guidance. In the following analysis, the hybrid guiding LCPCF was characterized by having the background refractive index of $n_b = 1.6$ and the diameter of the cylindrical rod of $d = 0.4\Lambda$. Similarly, the NLC was assumed to be nematic E7, which has an ordinary and extraordinary refractive index $n_o = 1.52$ and $n_e = 1.75$, respectively.

Fig. 4.16 shows the gap map for the PC cladding containing NLC with optic axis aligned transversely along the y direction. Since the symmetry of the unit cell is broken by the anisotropy, a greater portion of irreducible Brillion zone (IBZ) as shown in the inset figure is needed for the calculation [112]. As demonstrated by Eqs.(4.10) and (4.11), the band structure can be viewed as an overlap of gap regions of E_x and E_y . For comparison, Fig. 4.17 shows the bandgap structures of E_x and E_y which are evaluated by analyzing the gap maps of the PC claddings with $\epsilon_a = \text{diag}(n_o^2, n_o^2, n_o^2)$ and $\epsilon_a = \text{diag}(n_e^2, n_e^2, n_o^2)$, respectively. A direct comparison of Fig. 4.16 and Fig. 4.17, illustrates the formation process for the band structure of hybrid guiding anisotropic PCF. Above the radiation line of E_y , both polarization components are guided by TIR. In the region

between two radiation lines, the guiding mechanisms for two polarization components are different: E_x is guided by index-guiding effects, whereas E_y is guided by bandgap effects. In the shaded region below the radiation line of E_x , E_y is guided by bandgap effects; whereas the PC cladding no longer supports the guidance of E_x . Obviously, since the core line of $n=1.6$ crosses the bandgaps of E_y and lies within the index-guiding region of E_x , PBG-guiding and TIR can act together to confine light in the anisotropic PCF for E_y and E_x , respectively.

Fig. 4.16: Gap map of the PC cladding with optic axis of NLC inclusions along y direction. Inset figure: IBZ.

Fig. 4.17: Gap maps of E_x and E_y which correspond to the band structure of the PCs with $\epsilon_a = \text{diag}(n_o^2, n_o^2, n_o^2)$ and $\epsilon_a = \text{diag}(n_e^2, n_e^2, n_o^2)$, respectively.

Fig. 4.18 shows the modal dispersion curves of guided modes as a function of the wavelength. Six layers of NLC inclusions were used in the simulation in order to enhance the confinement. The pitch of the hybrid-guiding anisotropic PCF was chosen to be $2.6\mu\text{m}$ in order to shift the central wavelength of primary bandgap of E_y to 1550nm . The concept of hybrid guiding is further proved by the simulation results. As shown by the curve with solid circles, the dispersion curve for the x -polarized mode is incessant in the whole wavelength range. Since the refractive index contrast along x -axis is small, x -polarized light exhibits endless single mode guidance. However, as noticed from the curve with solid diamonds, the dispersion curve for the y -polarized light is truncated by the PBEs. Similarly, due to the small refractive index contrast along the y -axis, only the y -polarized fundamental mode is found to be guided in the gray-shaded bandgap region.

Fig. 4.18: Dispersion curves of guided modes as a function of the wavelength for x and y polarizations.

The difference in the guiding mechanism for two orthogonal fundamental modes also manifests in their transmission spectra. Fig. 4.19 shows the transmission spectra for two polarization components after propagating through a 1-mm long PCF, respectively. As shown by the curve with solid circle in Fig. 4.19, the transmission spectrum for the x -polarized light exhibits monotonous decrement with wavelength. This result certainly can be expected from the observation of the dispersion curve as shown in Fig. 4.18. When the operating wavelength approaches the value of pitch, the effective index of the x -polarized fundamental mode comes close to the cladding index or radiation line, leading to a greater loss. The loss could be reduced by increasing the refractive index contrast between the background material and ordinary index of NLC. On the other hand, for the y -polarized light, one of the key signatures in the transmission spectrum is an approximately periodic spectral response with wavelength, arising from the bandgap

guidance [118]. The locations of the transmission minima are governed by the diameters and refractive indices of the high-index cylinders, which can be described analytically by use of an ARROW model. Based on the ARROW model, the locations of the transmission minima correspond to the cutoff wavelength of a single high-index cylinder in the cladding. The cutoff wavelengths for TM_{0l} , TE_{0l} , HE_{1l} , EH_{1l} , HE_{2l} and EH_{2l} modes in the individual anisotropy cylindrical inclusions, which has the dielectric tensor of $\epsilon_a = \text{diag}(n_e^2, n_e^2, n_o^2)$ are described by Eqs.(4.12) and (4.13). These simple equations could be used to estimate the locations of transmission minima in the transmission spectrum of the y -polarized light.

Fig. 4.19: Transmission spectra for x and y polarizations.

The fundamental modes for the x - and y -polarized light adopt distinctive characteristics at different wavelengths in the transmission spectra. The mode intensity of

the x - and y -polarized fundamental modes at the wavelength of 780nm, 988nm and 1550nm are illustrated in Fig. 4.20. It shows that the x -polarized fundamental mode has a similar distribution across the whole wavelength range. The only difference is that the x -polarized light becomes less confined with the increment of wavelength. This aspect gives rise to a greater loss as the wavelength increases, which is consistent with the observation in Fig. 4.19. In contrast, a great difference is found between the mode fields in the transmission maxima and minima of the transmission spectrum for the y -polarized fundamental modes. Near the edges of transmission minima as shown in Fig. 4.20(e), the y -polarized fundamental mode has the characteristic of strong resonance in the high-index cylinder, which results from the resonance of high-index cylinders with the core mode and consequently causes light relayed outwards laterally. At the wavelength corresponding to the transmission maxima as shown in Fig. 4.20(d) and Fig. 4.20(f), the high-index cylinders are in antiresonance with the core mode. Light in the y polarization is thus rejected and confined in low-index core region. It is the specific feature in the modes that leads to a periodic spectral response with wavelength for the y -polarized light.

Fig. 4.20: Mode intensity of x-polarized fundamental modes at the wavelength of (a) 780nm, (b) 988nm and (c) 1550nm and of y-polarized fundamental modes at the wavelength of (d) 780nm, (e) 988nm and (f) 1550nm.

Their difference in the guiding mechanisms opens up a large degree of freedom in optical waveguide design, which may not be achieved in an isotropic PC structure. One of the potential applications for the hybrid guiding anisotropic PCF is the design of high-birefringence (Hi-Bi) fiber devices. Fig. 4.21 shows the modal birefringence for a range of wavelength by $B(\lambda) = |n_{eff}^x - n_{eff}^y|$. Numerical results show that the birefringence in the hybrid guiding anisotropic PCF can be easily achieved in the order of 10^{-2} . In particular, at the wavelength of 1550nm, the birefringence is approximately equal to 1×10^{-2} . The birefringence value in the calculations is conducted for the whole regions of the bandgap and it does not exhibit monotonic variation with wavelength. The birefringence experiences a decrement with wavelength followed by an increment in each bandgap. Therefore, high birefringence is able to be achieved at bandgap edges. The high

birefringence is also a result of the difference of guiding mechanisms. As shown in Fig. 4.18, for the x -polarized fundamental mode, the index-guiding mechanism restricts the dispersion curve in the region between the core line and the line representing cladding index. Since these two lines are close to each other, the effective index of the x -polarized fundamental mode is barely changed with wavelength. On the contrary, the dispersion curve of the y -polarized fundamental mode is confined in the shaded gap region below the core line. Since the gap region extends far below the core line, the effective index of the y -polarized fundamental mode varies significantly with wavelength. As a consequence, high birefringence in the order of 10^{-2} is easily obtained. Another potential application is to achieve single-polarization single-mode (SPSM) guidance. The inset figure of Fig. 4.21 shows the confinement losses difference between E_x and E_y within the wavelength range of $0.8\mu\text{m}$ to $1.2\mu\text{m}$. The wavelength range for SPSM operation varies with the length of the fiber. For example, if 20dB contrast is required to produce SPSM, the wavelength for SPSM guidance ranges from $0.92\mu\text{m}$ to $1.08\mu\text{m}$ for a 1-cm long PCF.

Fig. 4.21: Modal birefringence as a function of the wavelength. Shaded region represents the wavelength range outside the bandgaps of E_y . Inset, difference of the confinement losses of E_x and E_y within the wavelength range of $0.8\mu\text{m}$ to $1.2\mu\text{m}$

4.5 Hollow core anisotropic PBGFs ($n_b > n_e$ and $n_b > n_o$)

Till now, the guiding mechanism of the PC microstructure with $\varepsilon_b < n_o^2 < n_e^2$ has been investigated and can be appreciated by considering the resonant condition of a single NLC cylindrical rod. In particular, if the core is also made of the background material, the PBEs of PBG-guiding wavelength ranges can be approximated by the cut-offs of the NLC cylindrical rod based on an ARROW model. Moreover, the microstructure with $\varepsilon_b > n_e^2 > n_o^2$ is similar to the conventional air-silica structure. By intuition, the resonant conditions of the high-index nonsilica web have an impact on the formation of the band structure. However, unlike the PC microstructure with $\varepsilon_b < n_o^2 < n_e^2$, the cut-offs of the high-index nonsilica web are unable to be evaluated analytically. Therefore, numerical

schemes are necessary for the estimation of the locations of the bandgaps. Finally, the microstructure with $n_e^2 > \epsilon_b > n_o^2$ can only be realized in an anisotropic PC structure, where the guiding principles for two polarization components are expected to be distinguished. In the following, the band structure of the PC with $\epsilon_b > n_e^2 > n_o^2$ is investigated.

It is worth mentioning that the anisotropy of material can modify the symmetry properties of anisotropic PCs and thus the irreducible Brillouin zone (IBZ) varies with the alignment of NLC. In the following simulations, the microstructures of PC claddings are characterized by having the background refractive index of $n_b=2$ and the diameter of the cylindrical rod of $d=0.9\Lambda$. The dielectric tensor ϵ_a is determined by the alignment of NLC, which is assumed to be E7 and has an ordinary and extraordinary refractive index $n_o=1.52$ and $n_e=1.75$, respectively.

The gap map for the PC cladding containing NLC with optic axis aligned longitudinally along z direction is discussed in Section 4.2.2. According to Fig. 4.3 and Fig. 4.5, the presence of material anisotropy barely alters the bandgap structure of the isotropic PC cladding. Furthermore, assuming the entire air region, including the core and cladding of a nonsilica/air hollow-core PBGF, is filled with the material with refractive index equal to n_o , the PBG-guiding wavelength ranges, which are the spans where the core line crosses the gap regions, are found to satisfy a refractive index scaling law, which is described by Eq.(4.7).

Fig. 4.22 shows the gap map for the PC cladding containing NLC with optic axis aligned transversely along y direction. Since the symmetry of the unit cell is broken by the anisotropy, a greater portion of IBZ as shown in the inset figure is needed for the calculation. In this situation, the dielectric tensor of the cylindrical rod takes the form of $\epsilon_a = \text{diag}(n_o^2, n_e^2, n_o^2)$. As demonstrated by Eqs.(4.10) and (4.11), the formation of the bandgaps can be viewed as an overlap of gap regions of E_x and E_y , which are evaluated by analyzing the gap maps of the PC claddings with $\epsilon_a = n_o^2$ and $\epsilon_a = \text{diag}(n_e^2, n_e^2, n_o^2)$, respectively. Furthermore, the evaluation of the band structure of E_y can be simplified as a PC cladding with $\epsilon_a = n_e^2$. As a consequence, light of x or y polarizations can be considered to sense two different microstructures which have isotropic inclusions with refractive indices equal to n_o and n_e , respectively. Fig. 4.22(b) shows the bandgap structures of E_x and E_y which are evaluated by analyzing the gap maps of the PC claddings with $\epsilon_a = n_o^2$ and $\epsilon_a = n_e^2$, respectively. By comparing Fig. 4.22(a) with (b), it is easy to identify some practically interesting guiding regions. Above the radiation line of E_y , it is a region where index-guiding is able to be achieved for both E_x and E_y . Between two radiation lines, the guidance mechanisms for two polarization components are different: E_x is guided by index-guiding effects, whereas E_y is guided by bandgap effects. Under the radiation line of E_x and above the line representing $n = n_e$, both E_x and E_y exhibit the behavior of bandgap guidance and the absolute gap structure is determined by the overlap of the gap regions. In particular, it is interesting to examine the region below the line representing $n = n_e$, where the PC cladding no longer supports E_y by either

PBG-guiding or index-guiding. Therefore, only one polarization component, namely E_x , can be guided by the bandgap effects. Obviously, the demonstrated band structures in Fig. 4.22(a) and (b) are quite similar excepting small deviations, which indicate features that specifically from the vector nature of the electromagnetic field. Clearly, a similar refractive index scaling law can be also found under this approximation. Assuming a nonsilica/air hollow-core PBGF is filled with NLC orientated along y direction, the PBG-guiding wavelength ranges for E_x and E_y , satisfy:

$$\lambda/\Lambda = C_1 \sqrt{n_b^2 - n_o^2} \quad \text{for } E_x \quad \text{and} \quad \lambda/\Lambda = C_2 \sqrt{n_b^2 - n_e^2} \quad \text{for } E_y \quad (4.14)$$

where C_1 and C_2 are constants, respectively.

(a)

(b)

Fig. 4.22: (a) Gap map of the PC containing NLC with optic axis aligned along y direction. Inset figure: IBZ. (b) Approximated gap maps of E_x and E_y which correspond to the band structure of the PC claddings with $\epsilon_a = n_o^2$ and $\epsilon_a = n_e^2$, respectively.

4.6 Chapter Summary

The bandgap structures of anisotropic PBGFs have been investigated theoretically. Two general theoretical models are proposed to investigate the effects of refractive index scaling and NLC orientation on the bandgap structure. Based on these two models, the variations of bandgaps can be predicted by simple analytical formulas without tedious numerical work. In particular, three different types of anisotropic PBGFs have been investigated. The anisotropic PBGFs are grouped according to core and cladding compositions with $n_b < n_o < n_e$, $n_e > n_b > n_o$ and $n_b > n_e > n_o$, respectively. The corresponding bandgap structures have also been explored. As it has been shown that NLCs could act as an optical amplifier of protein-ligand bindings, the proposed theoretical model and detailed analysis of the corresponding bandgap structures could provide a simple guide for the design of novel anisotropic PBGFs based biochemical sensors.

Chapter 5

Photonic Bandgap Fibers based Biochemical Sensors

5.1 Introduction

The theoretical models for isotropic and anisotropic PBGFs have been demonstrated in Chapter 3 and Chapter 4, which offer the principles of design for realizing novel PBGFs based biochemical sensors. In this Chapter, three types of PBGFs based biochemical sensors will be demonstrated, with the aid of those models. In Section 5.2, a solid-core PBGF is proposed to measure the refractive index, which is larger than that of the silica. The sensing principle is based on the antiresonant reflecting optical waveguide (ARROW) model. In Section 5.3, a hollow-core PBGF is proposed to measure the refractive index which is smaller than that of the silica. The proposed sensing mechanism is based on the detection of the wavelength shift of the photonic-band-edge (PBE) due to the change of the refractive index inside the holey region of the PBGF, which has been investigated based on refractive index scaling laws. Since a bioactive layer can be immobilized on the inner surface of the holey region of the PBGF, the design of a PBGF based biosensor reactive to a specific bio-chemical agent is a logical extension. The proposed theoretical models are not limited within the range of refractive index based biochemical sensors.

They can also be extended to be designed as evanescent wave biosensors. In Section 5.4, a hollow-core PBGF is proposed for the measurement of the fluorescent dye labeled DNA oligo solutions. The performance of the hollow-core PBGFs based sensors can be estimated by using the refractive index scaling laws, which greatly simplifies the analysis procedures. A chapter summary is presented in Section 5.6.

5.2 Solid-core PBGFs for measuring high refractive index

5.2.1 Introduction

Generally speaking, the measurement range of refractive index of the conventional fiber-optic biochemical sensors is restricted below that of silica, which is around 1.45 [4, 5]. Recently, the family of fiber-optic biochemical sensors is enlarged, since the first photonic crystal fibers (PCFs) were demonstrated by Knight et al. Particularly, one way to realize PBGFs is to infiltrate the air holes of solid-core PCF with high-index fluid [118, 142, 143]. As the core defect becomes a low-index region after filling process, the guiding mechanism of the fibers also changes from index guiding to photonic bandgap guiding. In Section 4.2, the ARROW model has been used to explain the guidance mechanism of such fibers. According to the ARROW model, the locations of stop bands, which appear as transmission dips in the transmission spectrum, are determined by the resonance of an individual high-index rod, which coincide with the cut-offs of the guiding modes in the rods. As the refractive index inside the air holes of such fiber

directly modify the cut-offs of the guiding modes in the rods, the wavelengths of the transmission dips shift with the change of refractive index. Since the locations of the transmission dips are strongly dependent on the refractive index of the infiltrating liquid, this type of solid-core PBGFs offers the potential of the measurement of the liquid or biochemical solutions with high refractive index.

5.2.2 Experimental investigation of the performance

The schematic diagram of the experimental setup is shown in Fig. 5.1. Two ends of a 30cm solid-core PBGF were mounted in modified V-groove mounts in order to keep the fiber submerged during the measurements. Light from a supercontinuum source was guided using a single-mode fiber SMF-28 which in turn launched into the core of the solid-core PBGF via butt coupling. The transmitted light after the solid-core PBGF was guided using another section of SMF-28 via butt coupling again and then measured by using an optical spectrum analyzer (OSA). The butt coupling method aligns the ends of two fibers closely in order to achieve low loss transmission. The alignment was achieved by mounting the fibers on the platforms of two translation stages. The translation stage is a tunable moving platform. Rotating the screw or micrometer pushes the platform moving towards x, y and z directions. The alignment can thus be controlled precisely. The measured transmission spectra span from 1 μ m to 1.7 μ m. The air holes of the solid-core PBGFs were filled with the liquid by capillary force. Without specific equipments, this process was achieved by inserting one side of the fiber inside the liquid while leaving the

other side in the air. It takes 20 minutes to fill a 20 cm long PCF. The length of the liquid inside the fiber does not affect the locations of the transmission dips, which are most of concern. It only modifies the magnitudes of the transmission dips. As the requirement for antiresonant guiding is $n_a > n_b$, the refractive index of the analytes must be larger than that of silica.

Fig. 5.1: Schematic diagram of the experiment setup. (SC light source: Supercontinuum light source; OSA: optical spectrum analyzer; PBGF: photonic bandgap fiber).

The refractive index liquid (Cargille Labs) which have the refractive indices of 1.52 and 1.64 were used to fill the fiber. Fig. 5.2 and Fig. 5.3 show the transmission spectra after filling with refractive index liquid with index of 1.52 and 1.64, respectively. With the aid of these two refractive index liquid, it is able to demonstrate the transmission dips which are derived from LP_{ml} modes ranging from LP_{31} to LP_{14} modes. The modal cut-off wavelengths are evaluated by considering the material dispersion of refractive index

liquid and silica. They are demonstrated as dot lines and dash lines in Fig. 5.2 and Fig. 5.3. Clearly, the modal cut-off wavelengths show a good agreement with the locations of the transmission dips in the transmission spectra. In addition, it is observed that LP_{ml} ($m \leq 4$) modes take part in the formation of the transmission dips, which has not been demonstrated by the previous numerical work. The higher-order modes, such as LP_{51} and LP_{61} , related stop bands are not observed in the transmission spectra. This might be the reason that their transmission dips are too narrow and thus cannot be observed in the experiment.

Fig. 5.2: Transmission spectrum of the solid-core PBGF with ambient refractive index of 1.52.

Fig. 5.3: Transmission spectrum of the solid-core PBGF with ambient refractive index of 1.64.

Another observation is that stop bands splitting does not appear in the transmission spectra for $LP_{ml} (m \geq 3)$ related stop bands. This is for the reasons that the splitted cut-offs of $LP_{ml} (m \geq 3)$ modes are too close to each others. Therefore, the corresponding stop bands or transmission dips can overlap and form wider stop bands or transmission dips. As a result, according to Fig. 5.2 and Fig. 5.3, the widths of the transmission dips derived from $LP_{ml} (m > 2)$ modes are nearly equal to that of the adjacent transmission dips derived from $LP_{ml} (m \leq 2)$.

Fig. 5.4: Wavelength shifts of transmission dips. Lines represent the analytical results.

For a small refractive index change of Δn_a , the wavelength shift of $\Delta \lambda_{ml}$ can be obtained by taking derivatives of both sides of Eq.(3.2), which gives

$$\frac{\Delta \lambda_{ml}}{\Delta n_a} = \frac{n_a}{n_a^2 - n_b^2} \cdot \lambda_{ml} \quad (5.1)$$

The sensitivity to the refractive index change is measured by using refractive index liquid with refractive index intervals of 0.02. Fig. 5.4 shows the wavelength shifts of the transmission dips when the refractive index changes around 1.64. Each step of refractive index change is 0.01RIU. The lines which represent the analytical results evaluated by Eq. (5.1) show a good agreement with the experimental results. It should be noted that Eq. (5.1) is only valid for a small refractive index change. An example was demonstrated in Fig. 5.4, where experimental results (symbols) show a good agreement with analytical results (lines). However, for large refractive index change of 0.12 from 1.52 to 1.64, the wavelength shifts of the bandgaps must be determined by Eqs. (3.1) and (3.2). The lower

order transmission dips or the transmission dips which are located at longer wavelengths have a larger wavelength shifts. For example, the LP_{32} derived transmission dips have a wavelength shift of 45nm in response to the refractive index change of 0.01RIU; whereas the LP_{23} and LP_{04} derived transmission dips have a wavelength of 36nm in response to the refractive index change of 0.01RIU. The minimum detectable refractive index is dependent on the minimum detectable wavelength shifts. Assuming that the OSA can resolve 50pm wavelength shift, the minimum detectable refractive index is in an order of 1×10^{-5} RIU. As the temperature coefficient of the liquid is $-4.59 \times 10^{-4}/^{\circ}\text{C}$, it also requires thermal stability within 0.02°C .

In addition to measure the refractive index change, such sensors can also be potentially useful for humidity and gas sensing by filling a polymer inside the air holes, as the refractive index of the polymer changes with the exposure to a water vapor or to a specific gas. Examples of such polymers are polyethylene oxide for humidity sensing and ferrocene-based polymers for various gas sensing [144, 145]. The refractive indices are higher than that of silica, therefore an antiresonant guiding PCF is formed after filling.

5.3 Hollow-core PBGFs for measuring of low refractive index

Hollow-core PBGFs are characterized by having a hollow core which is surrounded by a pattern of micrometer-sized air holes along the entire length of the fiber [79]. According to the theoretical model and numerical analysis in Chapter 4, the locations of

the transmission windows obey the refractive index scaling law. It therefore offers the possibility of detecting the change of refractive index by measuring the wavelength shifts of the PBE. In addition, the design of a hollow-core PBGF based biosensor reactive to a specific biochemical agent is possible by immobilizing a bioactive layer on the inner surfaces of the holey regions.

5.3.1 Experimental investigation of the performance

Experiments were conducted using hollow-core PBGFs as non-specific biochemical sensors. The bare hollow-core PBGFs without chemical treatment were used as the transducer. In this regard, the hollow-core PBGF biochemical sensor could be used to measure the concentration of a known chemical solution, or to distinguish a target chemical from a few known chemicals.

Fig. 5.5: Schematic diagram of the experiment setup. (SC light source: Supercontinuum light source; OSA: optical spectrum analyzer; PBGF: photonic bandgap fiber).

The schematic diagram of the experimental setup is shown in Fig. 5.5. The hollow-core PBGF (Crystal-Fiber HC-1550-02) used in the experiment has a cladding pitch of $3.8\mu\text{m}$, a core diameter of $10.9\mu\text{m}$ and center operating wavelength of 1550nm . Two ends of the PBGF were mounted in modified V-groove mounts in order to keep the fiber submerged during the measurements. Light from a supercontinuum (SC) source (KOHERAS SuperK Red) was guided using a single-mode fiber SMF-28, which in turn launched into the core of the hollow-core PBGF via butt coupling. The transmitted light after the hollow-core PBGF was guided by using another section of SMF-28 via butt coupling again and then measured by using an OSA (ANDO AQ6317B). As a light source, the SC source provided an ultra broad flat spectrum from 600nm to 1750nm which had the same wavelength range as the OSA. The holey region of the hollow-core PBGF was filled with the biochemical solution by capillary force. Based on calculations using the Navier-Stokes equations for the rate of liquid flow into a circular hole, the time required to fill a 20 cm long hollow-core PBGF with aqueous solution was around 10min and this was confirmed experimentally [146]. It was also possible to apply pressure or temperature in order to reduce the filling time to less than 4min . All the experiments were carried out in a controlled environment, where the effect of temperature variation can be ignored.

Fig. 5.6: Transmission spectra of (a) 20cm and (b) 50cm hollow-core PBGFs without filling.

Fig. 5.6(a) and (b) show the transmission spectra for two hollow-core PBGFs, which have the lengths of 20cm and 50cm, taken before the filling process. In both cases, two bandgaps are observed: The primary bandgap has a center operating wavelength of 1550nm and the secondary bandgap has a center wavelength of 1100nm. The variation of the length of the fiber does not shift the position of the bandgap since the bandgap is only determined by the microstructure in the transverse direction. However, the loss outside the bandgaps shows a strong dependence on the length of the hollow-core PBGF. Increasing the length of the fiber can increase the loss outside the bandgaps, while the transmission inside the bandgaps is almost not altered. Intuitively, a longer hollow-core PBGF is suitable for achieving high transmission contrast and thus is not vulnerable to the loss, whereas a shorter hollow-core PBGF is preferred to design a compact sensor probe for lab-on-chip system. In the following demonstrated experiments, all the fiber

samples were kept at 20cm long.

Fig. 5.7: Normalized transmission spectra taken (a) before and (b) after filling with water.

The normalized transmission spectra taken before and after the filling of water are plotted together and shown in Fig. 5.7(a) and (b), respectively. The transmission spectrum before the filling process spanned from 1400nm to 1800nm. After filling process, the transmission spectrum ranged from 600nm to 1162nm. This range was broader than the prediction of the scaling law which had a range from 790nm to 1020nm. This is because the scaling law is based on the scalar waveguide approximation which is accurate for small index contrast. Another observation is that there are several loss dips in the transmission window after filling process. The loss phenomenon is believed to result from the absorption and attenuation of visible and near-infrared light in water [147]. It is worth mentioning that the water has several specific discrete absorption lines [147, 148]. Strong water absorption bands occur at wavelengths around 2500 nm, 1950 nm and 1450

nm, with weaker absorption around 1220 nm and 970 nm, and three additional sets of water-vapor absorption lines near 930, 820, and 730 nm, all of these are located in the infrared spectrum [147, 148]. The absorption line of 1220nm is near the PBE, it may corrupt the bandgap and thus alter the PBE.

Fig. 5.8: (a) Normalized transmission spectra of the hollow-core PBGF with three different ambient refractive indices ranging from $n_a=1.35$ to $n_a=1.39$. (b) Wavelength shift of the falling PBE plotted as a function

of ambient refractive index n_a

Refractive index liquid (Cargille Labs) which have the refractive indices of 1.35, 1.37 and 1.39 were used to determine the sensitivity of the refractive index measurement. The corresponding calibrated refractive index accuracy for each liquid is ± 0.0002 RIU. Fig. 5.8(a) shows the normalized transmission spectra taken after filling the fiber with liquid. For each measurement, a new fiber was used in order to avoid the possibility of contamination that might affect the measurements. The wavelengths of rising PBEs were unable to be recorded since they were out of the operating range of the SC source and OSA. Two conclusions can be drawn from Fig. 5.8(a). Firstly, the transmission window shifts to a shorter wavelength when the refractive index of the liquid increases. When the refractive index varies from 1.333 to 1.39, the falling PBE has a shift from 1159nm to 882nm. Secondly, with an increase of the refractive index, the transmission window becomes lossier. This is caused by the low index contrast between the solution and silica reducing the confinement of the light. In Fig. 5.8(b), the wavelengths of the falling PBEs are plotted as a function of the ambient refractive index (n_a). The wavelengths of the falling PBEs at $n_a=1.35$, 1.37 and 1.39 are fitted by using Eq.(3.7), where $n_a=1.333$ is ignored since the falling PBE is possibly distorted by the absorption of water at the wavelength of 1220nm. The large discrepancy between the experimental results at $n_a=1.333$ and the fitted curve further proves this assumption. This might be avoided by choosing a hollow-core PBGF that has a different center operating wavelength, for example 1060nm. On the other hand, for other refractive indices, the experimental results

show good agreement with the analytical results with a correlation coefficient of $R^2 = 0.9941$, since there are no strong absorption lines in the vicinity of their PBEs. The minimum detectable refractive index change depends on the demodulation technique and operating refractive index. For a small refractive index change of Δn_a , the wavelength shift of $\Delta\lambda$ can be obtained by taking derivatives of both sides of Eq.(3.7), which gives

$$\frac{\Delta\lambda}{\Delta n_a} = \frac{n_a}{n_b^2 - n_a^2} \cdot \lambda \quad (5.2)$$

In Fig. 5.8, it can be seen that the PBE has a blue shift of $\sim 110\text{nm}$ for $\Delta n_a = 0.02$ at $n_a = 1.35$, which can be estimated by Eq. (5.2). A RIU sensitivity on the order of $2 \times 10^{-6}\text{RIU}$ should be obtained by using the demodulation technique, which can achieve a resolution of about 0.01nm for wavelength detection.

The liquid has the refractive index ranging from 1.300 to 2.31 [149]. Therefore, the measurements were conducted in the range from 1.300 to 1.45. However, for the refractive index larger than 1.39, the refractive index contrast between silica and liquid is small and the whole waveguide becomes lossy in the experiment. As a consequence, only the results with refractive index ranging from 1.33 to 1.39 were demonstrated.

5.3.2 Discussion

The hollow-core PBGF based sensor has so far only been tested in applications as a non-specific biosensor, which shows its potential to measure the concentration of a specific solution. The use of the hollow-core PBGF sensor to distinguish different solutions appears possible assuming that a biorecognition element is immobilized on the

inner surface of the holey region of the fiber by physical or chemical methods. It has been demonstrated that goat anti-human IgG (antibody) can be used as a biorecognition element to detect a specific biomolecule, human IgG (antigen). This concept may be used for a variety of biodetection events by using different biorecognition elements, such as various enzyme and antibodies.

Fig. 5.9: Simplified model of a hole in the cladding after the formation of a biolayer.

The sensitivity to the concentration variation can be estimated by considering the formation of the biolayer on the inner surface of the holey region. In order to simulate the biolayer effect, a simplified three layer model of a hole in the cladding for evaluating the wavelength shift of PBEs is proposed, as shown in Fig. 5.9. The three layers include: (1) background material with a refractive index n_b ; (2) biomolecular layer with refractive index n_F and thickness d_F , and (3) bulk solution region with a refractive index of n_a and diameter of d_a ($d_a = d - 2d_F$). When specific binding occurs, both the thickness d_F and the

refractive index n_F of the biolayer change. It is really difficult to predict the exact final values of the thickness d_F and the refractive index n_F after the binding reaches equilibrium or saturation. However, it is possible to investigate two extreme cases for estimation of the corresponding sensitivity.

Fig. 5.10: Wavelength shift of the falling PBE as a function of biolayer thickness.

The first situation is based on the assumption that the refractive index of the biolayer n_F is constant, whereas its thickness changes during binding. The shifts of the wavelength of the PBEs can be evaluated by using plane wave methods (PWM) assuming that $n_F=1.45$ and $n_a=1.333$. The hollow-core PBGF in the simulation has a cladding pitch Λ of $3\mu\text{m}$ and hole diameter d of $2.85\mu\text{m}$ which has a transmission spectrum spanning from 800nm to 1100nm when $n_a=1.333$ and $d_F=0$. The shift in the wavelength of the falling PBE with respect to the thickness d_F is demonstrated in Fig. 5.10. The wavelength shift is a linear function of the thickness of the biomolecular monolayer with a slope of

$d\lambda/d(d_F)=0.186$. The maximum thickness is around 5nm for a typical biosensor. A small variation of 0.054nm in the thickness d_F can be detected when a wavelength shift of 0.01nm can be detected. According to Ref.[54], this result corresponds to a surface coverage change $\Gamma_{\min} \approx 3.5\text{ng/cm}^2$ for the detection of proteins, which is on the same order as other optical methods, such as the SPR method (gold film: $\sim 11\text{ng/cm}^2$, silver films: $\sim 2.5\text{ng/cm}^2$) and integrated optical (IO) sensors with grating couplers ($\sim 0.4\text{ng/cm}^2$) [52].

Fig. 5.11: Wavelength shift of the falling PBE as a function of the biolayer refractive index

The second case is based on the assumption that the thickness d_F is kept constant at 5nm, whereas the refractive index n_F is varied from 1.333 to 1.45. The wavelength shift of the falling PBE is plotted as a function of n_F ($n_a < n_F < n_b$) in Fig. 5.11. A linear relationship is observed with a slope of $d\lambda/d(n_F)=7.75\text{nm/RIU}$. Assuming a wavelength shift of 0.01nm can be detected, a small refractive index variation $1.2 \times 10^{-3}\text{RIU}$ can be measured. The minimum detectable surface coverage $\Gamma_{\min}$ can be evaluated by using de

Feijter's formula [147].

$$\Gamma_{\min} = d_F \cdot \frac{n_F - n_a}{dn/dc} \quad (5.3)$$

where c is the concentration of the molecules and dn/dc is the corresponding refractive index increment. For example, the refractive index increment of proteins varies remarkably little from one protein to another, and has a typical value of $dn/dc \approx 0.18 \text{ ml/g}$. Therefore, the minimum detectable surface coverage $\Gamma_{\min}$ is 3.5 ng/cm^2 . To take human IgG as an example, the analyte concentration required to obtain this minimum surface coverage after equilibrium is on the order of 0.1 nmol/L according to Ref.[150]. It should be noted that this sensitivity might be enhanced by modifying the size of the holes, which requires for further investigation.

The main advantage of the hollow-core PBGF sensor is that it provides high sensitivities for refractive index measurements, which results from the large wavelength shift of PBEs with respect to refractive index change. The sensitivity to the concentration variation is estimated to be around 0.1 nmol/L for human IgG detection. In addition, the design rules are simple as described by Eq.(3.13) and Eq.(5.2). This device is also robust since there is no need for the removal of the cladding, which is commonly required in fiber-based SPR system. Although silica is the most commonly used material for fabricating PBGF, a polymer, such as polymethylmethacrylate (PMMA), is another attractive option [151]. One of the advantages of polymer based fibers over silica ones is, that many biological substances are more compatible with polymers than with silica. The

preparation of the air holes with the deposition of a sensor layer should be easier and hence more reliable and reproducible. The PBGF biosensor also has the merit of small volume sample consumption, which is less than 1 μL .

5.4 Evanescent Wave Sensing

Over the last two decades, optical fibers and waveguides have been widely used for developing optical biosensors [64]. Evanescent wave biosensors are based on interaction of the analyte species with the electromagnetic wave, which extends from the surface of the light-guiding waveguides [2, 146]. The interaction between evanescent wave and analytes produces absorption, spontaneous emission, stimulated emission and Ramon scattering, which have been used extensively both in a planar waveguide and in fiber geometry. The efficiency of this kind of biosensor is determined by sufficient interaction length and large overlap between light and fluorescent dye labeled analytes. It is also more efficient as the overlap between the incident light probe and the collected optical response is maximized. Approaches used to realize large overlap between light and analytes are based on reducing the radius of the fiber, including unclad, partially clad, and D-shaped forms. The removing of cladding causes the sensing devices fragile. Moreover, the mismatch between the clad region and unclad region bring about large loss. More in particular, for fluorescence emission measurement, which needs to couple fluorescence emission from the surface back into the fiber, the efficiency is greatly decreased.

Emergence of PCFs, especially hollow-core PBGFs, opens up new opportunities for

novel evanescent-wave biosensor design, which could solve the problems encountered in the conventional biosensors [13, 14]. Hollow-core PBGFs comprise an air core with a cladding consisting of a two dimensionally periodic array of air inclusions in silica. As stated by their names, hollow-core PBGFs guide light in the air core within certain wavelength ranges, which are named as bandgaps and manifest as transmission windows in the transmission spectrum. Particularly, when aqueous solution is filled in the holey region of hollow-core PBGFs, the transmission windows have a blue shift and could cover the wavelength ranges of fluorescence spectra [152, 153]. The strong confinement of light in the aqueous core could provide a strong interaction between light and analytes. More in particular, for fluorescence emission measurement, since the incident light and collect optical responses are both confined in the core, their overlap is maximized [146, 151].

5.4.1 Theory and Simulation results

The structure of the hollow-core PBGF used in the experiment is demonstrated in Fig. 5.12, which is designed to guide light in the wavelength range from 1400nm to 1800nm. Following the previous designations, the PC cladding can be characterized by four parameters: hole-to-hole distance Λ , hole diameter d , refractive index n_a in the holey regions and n_b in the silica regions. The diameter of the hollow core is D .

Fig. 5.12: Hollow-core PBGF with air holes arranged in a triangular lattice. Black regions represent air.

According to the Beer-Lambert's Law, a crucial factor determining the amount being absorbed is the absorbance $A(\nu)$, which is defined as [2, 146]

$$A(\nu) = \log_{10} \left(\frac{I_0(\nu)}{I(\nu)} \right) = \varepsilon(\nu) c L_{eff} \quad (5.4)$$

where $I_0(\nu)$ and $I(\nu)$ are the intensities before and after the sample, respectively; ν is the frequency of light. $\varepsilon(\nu)$ is called the molar extinction coefficient at frequency ν . c is the concentration of the sample. L_{eff} is the effective optical path defined by the length of the sample through which the light travels, supposing hundred percent overlap between light and sample. The transmission T can be simply written as

$$T(\nu) = 10 \log_{10} \left(\frac{I_0(\nu)}{I(\nu)} \right) = 10 A(\nu) \quad (5.5)$$

For evanescent-wave biosensors, only part of the guiding light interacts with the sample. Therefore, the effective optical path length is determined by the fiber length l and the

sensitivity coefficient r , which is given by

$$L_{eff} = rl \quad (5.6)$$

The sensitivity coefficient r is an important parameter in quantifying the fiber efficiency, and has the value of $r = (n_r/n_{eff})f$, where n_r is the refractive index of the sensed material and n_{eff} is the modal effective index. The percentage of energy in the holes f is described as

$$f = \frac{\int_{sample} \text{Re}(E_x H_y^* - E_y H_x^*) dx dy}{\int_{total} \text{Re}(E_x H_y^* - E_y H_x^*) dx dy} \quad (5.7)$$

where $E_{x/y}$ and $H_{x/y}$ are the electric and magnetic fields along x and y directions.

The performance of the evanescent wave sensor is mainly determined by the modal effective index as well as the percentage of energy in the holes. Tedious numerical simulation is crucial to evaluate these two parameters in the conventional fiber design. This can be avoided for the hollow-core PBGFs by using refractive index scaling laws. The wave equation for the scalar field distribution in a hollow-core PBGF can be described in terms of normalized transverse coordinates $X=x/\Lambda$ and $Y=y/\Lambda$ and an index distribution function [126, 140, 154]

$$f(X, Y) = \begin{cases} 0 & \text{low index regions} \\ 1 & \text{high index regions} \end{cases} \quad (5.8)$$

$$\frac{\partial^2 \Phi}{\partial X^2} + \frac{\partial^2 \Phi}{\partial Y^2} + (v^2 f(X, Y) - w^2) \Phi = 0 \quad (5.9)$$

where $v^2 = \left(2\pi \frac{\Lambda}{\lambda}\right)^2 (n_b^2 - n_a^2)$ and $w^2 = \left(2\pi \frac{\Lambda}{\lambda}\right)^2 (n_{eff}^2 - n_a^2)$.

The refractive index scaling law can be described as follows: if n_a is varied, the

scalar field distribution can be kept unchanged, supposing that the normalized wavelength λ/Λ is adjusted so as to keep the value v and w invariant. In particular, the locations of the transmission windows after the hollow-core PBGF is filled with aqueous solution can be estimated by considering the invariant v . Supposing that the bandgaps originally at a wavelength λ_0 for an air-guiding hollow-core PBGF with $n_a=1$, after the fiber is filled with aqueous solution with $n_a=n_r$, it shifts to a new wavelength λ , which is given by

$$\lambda = \lambda_0 \left(\frac{n_b^2 - n_r^2}{n_b^2 - 1} \right)^{\frac{1}{2}} \quad (5.10)$$

As v and w is invariant, their ratio v^2/w^2 is also invariant. The modal effective index $n_{eff}(\lambda)$ at the wavelength λ after filling can thus be evaluated by the modal effective index $n_{eff}(\lambda_0)$ at the wavelength λ_0 before filling, which is given by

$$n_{eff}(\lambda) = \left(n_r^2 - \left(1 - n_{eff}^2(\lambda_0) \right) \left(\frac{n_b^2 - n_r^2}{n_b^2 - 1} \right) \right)^{\frac{1}{2}} \quad (5.11)$$

Since the scalar wave distribution is invariant when the bandgaps shift from a wavelength λ_0 to a wavelength λ , the percentage of energy in the holes at the wavelength of λ is equal to that at the wavelength of λ_0 , or

$$f(\lambda) = f(\lambda_0) \quad (5.12)$$

These equations provide simple tools for estimating the efficiency of hollow-core PBGF based biosensors by utilizing the parameters list on the manual of the products.

(a)

(b)

Fig. 5.13: Electric field distributions (a) at $\lambda_0=1.55\mu\text{m}$ before filling of pure water and (b) $\lambda=0.853\mu\text{m}$ after the filling of pure water.

In order to demonstrated this idea, Fig. 5.13(a) and (b) demonstrated the electric field distribution at $\lambda_0=1.55\mu\text{m}$ before filling of water and $\lambda=0.853\mu\text{m}$ after the filling of water. A full vectorial beam propagation method was used to evaluate the electric fields with the parameters of $\Lambda=3.8\mu\text{m}$, $n_b=1.45$, $n_r=1$ and $n_f=1.33$ before and after filling with water. As these two wavelengths satisfy the refractive index scaling law, their corresponding electric fields show no difference. The corresponding fractions of light propagating in the

air holes or samples are both around 96%. The corresponding modal refractive indices n_{eff} are 0.9881 and 1.3267 when $n_r=1$ and $n_r=1.33$, respectively, which also agree well with the refractive index scaling law described in Eq.(3.7). This greatly facilitates the design procedure of hollow-core PBGF based evanescent-wave biosensors.

5.4.2 Experimental investigation of the performance

The schematic diagram of the experimental setup is shown in Fig. 5.5. A 30cm hollow-core PBGF (Crystal-Fiber HC-1550-02) was used in the experiment with the holey region filled up with the Alexa Fluor 700-labeled DNA Oligo solution (Invitrogen) by capillary force. The Alexa Fluor 700 has an absorption maximum at 696nm with a molar extinction coefficient of $192,000\text{M}^{-1}\text{cm}^{-1}$.

According to the theoretical model and experimental results shown in Fig. 5.8, the wavelength shifts of the transmission windows obey the refractive index scaling law. Another issue is that the modal effective index n_{eff} and fraction of power residing in the holes f are related to the operating wavelength. However, as they show small variations across the wavelength ranges of the transmission windows, n_{eff} and f are assumed to be invariant across the wavelength ranges of the transmission windows. This greatly facilitates the design and analysis process.

Fig. 5.14 shows the transmission spectra of two 30cm hollow-core PBGFs, one filled completely with a $0.2\mu\text{M}$ Alexa Fluor 700 labeled DNA Oligo solution and one with pure water. The inset shows the derived absorbance with a maximum value of 1.06 at

$\lambda=696\text{nm}$. This could be evaluated by using Eq. (5.4) and refractive index scaling law. Since only a fraction of light propagates in the sample, the effective optical path length L_{eff} is introduced to describe the absorbance $A(\nu)$. As $L_{eff}=(n_r/n_{eff})fl$, the fraction of power f and the modal effective index n_{eff} should be known to obtain the value of L_{eff} . However, as described above, the refractive index scaling law provides a simple tool to evaluate these two parameters. The hollow-core PBGF used in the experiment has an effective mode index around 0.99 and fraction of light propagating in air around 95% at 1550nm. Assuming that these two parameters are invariant across the wavelength ranges of the transmission windows, after the fiber is filled with aqueous solution with $n_r=1.33$, the effective mode index is 1.3277 and the fraction of light propagating in the sample is 95%. As a result, the effective optical path length L_{eff} for a 30cm hollow-core PBGF is 28.6cm. Considering the molar extinction coefficient at 696nm of $192,000\text{M}^{-1}\text{cm}^{-1}$ and the concentration of $0.2\mu\text{M}$, the expected absorbance is 1.098, which is in good accordance with the measured value.

Fig. 5.14: Transmission spectra of two hollow-core PBGFs with a $0.2\mu\text{M}$ Alexa Fluor 700 labeled DNA solution (solid curve) and pure water for reference (dotted curve), respectively. Inset, derived absorbance in the sample containing the Alexa Fluor 700 labeled DNA Oligo solution.

Alexa Fluor 700-labeled DNA Oligo solutions which have the concentrations of $0.1\mu\text{M}$ and $0.05\mu\text{M}$ were also used to evaluate the sensitivity of the hollow-core PBGF. The corresponding derived absorbances are demonstrated in Fig. 5.15, which are in good agreement with the analytical results. The minimum detectable concentration is mainly limited by the minimum detectable absorbance. It has been demonstrated that the minimum detectable absorbance can be achieved to be $A=0.04$ [155]. Therefore, for a hollow-core PBGF with the length of 30cm, it offers the possibility of detecting Alexa Fluor 700 labeled DNA Oligo solution with concentration down to 7nM, provided that the reference spectra are accurate and stable. With a small sample volume consumption of only $1\mu\text{L}$, it offers the potential for the design of high sensitivity evanescent wave biosensors.

Compared with the solid-core PCFs based evanescent wave sensor which had evanescent field within the holes of 3.3% [155], the demonstrated hollow-core PBGFs have the advantages of large overlap between the light and the sample residing in the holey areas, which is 28.8 times larger. This provides a high efficiency for the evanescent wave biosensing applications. Fini has proposed a water-core PCF structure for biosensing applications, which is based on index-guiding mechanism [7]. Although it was possible to achieve 90% overlap between the light and samples, this method required selective filling technique to fill the hollow core with the sample rather than the whole holey regions. In addition, the analysis and design procedure needed tedious numerical work. A similar method was also proposed by selective filling the hollow core with sample solution, but the guiding mechanism was based on the bandgap guiding [156]. This method evidently experienced the same problems, including the selective filling process and the tedious numerical work. Another type of hollow-core PCF based evanescent sensor was demonstrated by filling the entire holey region with samples. Although the fiber structures and filling technique seem similar, the guiding mechanisms are totally different. In Ref. [146], light was guided through the silica in the entire cladding rather than the hollow core. In other words, light was not guided by bandgap effects. Therefore, only 5.2% fraction of power resides in the samples. This value was greatly smaller than the hollow-core PBGFs used in this experiment which has an overlap of 95%. In addition, as the light dissipates in the cladding, the loss is significantly large, which also introduces the difficulty into the spectral measurement.

Fig. 5.15: Absorption measurement for different concentrations of Alexa Fluor 700 labeled DNA solutions.

The success of hollow-core PBGFs is not limited in the evanescent wave sensing. As the hollow-core PBGFs provide a strong interaction between light and samples inside the holey regions. They are also ideal for the other sensing techniques, such as SPR and surface enhanced Raman techniques. Due to a large part of evanescent wave residing in the sample, only a short section of hollow-core PBGF which is 30cm is required to obtain high sensitivity. This greatly enhances the detection efficiency. In addition, this method does not require selective filling technique, which further offers the convenience for the practical applications.

5.5 Discussion

5.5.1 Effect of temperature variation

An important practical consideration is the temperature effect, which may limit the

minimum detectability of analyte. This is inevitable in the design of refractive index sensors and corresponding biochemical sensors. A liquid's temperature coefficient of refractive index can be expressed as the change in refractive index per °C, i.e. RIU/°C. It is always negative so that as temperature increases, refractive index decreases. Liquid temperature coefficients are usually so much higher than for solids that the user must know the temperature of a liquid to know its refractive index. With solids, temperature is less critical. It is sometimes advantageous to adjust the refractive index of a liquid by adjusting the temperature. Optical liquid with refractive indices less than 1.63 tends to have temperature coefficients of $dn/dT = -0.0003 \text{ RIU/°C}$ to -0.0004 RIU/°C , where T represents the temperature. Temperature coefficients for liquid with refractive indices above 1.63 and up to 1.70 tend to be about $dn/dT = -0.0005 \text{ RIU/°C}$ [157]. The refractive index variations due to the thermal effects certainly alter the locations of the transmission dips or transmission windows, which leads to the uncertainty of determining the refractive index. The temperature induced wavelength shifts could be estimated according to Eqs.(5.1) and (5.2). In these two equations, the refractive index variation Δn_a could be expressed explicitly as the function of temperature, i.e. $\Delta n_a = \frac{dn}{dT} \cdot \Delta T$. Therefore, both equations can be given as

$$\frac{\Delta \lambda}{\Delta T} = \frac{n_a}{|n_a^2 - n_b^2|} \cdot \frac{dn}{dT} \cdot \lambda \quad (5.13)$$

For example, given $\lambda = 1550 \text{ nm}$, $dn/dT = -0.0004 \text{ RIU/°C}$, $n_a = 1.33$ and $n_b = 1.45$, the wavelength shift is -2.47 nm/°C . Therefore, it is necessary to perform the experiment in a

temperature-controlled environment. On the other hand, it has been demonstrated that the evanescent wave is only intense at the silica-solution surface and vanishes completely after a short distance from the surface [158]. Therefore, the bandgaps are most likely to be influenced significantly by the refractive indices in close proximity to the inner surface of the holey region of the hollow-core PBGF, i.e. the layer of biomolecules deposited on the inner sides of the holes, rather than the average refractive index in the pores. This is expected to make the target specific biosensor more robust to variations of temperature, but this requires further investigation.

5.5.2 Reusage of PBGFs

Another important issue is the potential for the reuse of the PBGFs for multiple tests during semi-continuous on-line monitoring. For the demonstrated non-specific sensing system, the PBGFs can be cleaned with acetone and isopropanol. The filling and cleaning processes can be achieved with the aid of a pressure chamber. The PBGF based sensor can be developed for detecting specific targets, for example, by using an immobilized antibody biosensor. Regeneration of the PBGF sensor for the antibody-antigen detection is also possible since many techniques have been demonstrated to dissociate antibody-antigen complexes including pressure, electrical field and solvents [54]. The regeneration methods can thus follow those techniques commonly used in conventional fiber-optic biosensors.

5.5.3 Background humidity, contamination and pollution

The final concern comes from the background humidity, contamination and pollution, which may come from the accumulation of the residual antigen after several uses of the PBGF biosensor. These effects can be minimized by the re-treatment of the inner surface of the holey region of the fiber for further reuse. A typical procedure is to remove all the coatings (including antigen, antibody, cross-linking agents, and APTs) from the inner surface of the holey region by using acid treatment.

5.5.4 Other biochemical sensing applications

The biochemical sensing applications are not limited in the measurement of refractive index and fluorescent absorption spectrum as demonstrated. For example, it can be used to enhance the fluorescence sensing [156, 159]. Some research groups also try to deposit a metal layer on the inner surface of the PBGFs to design a SPR sensor or a SER sensor [160-163]. According to the previous analysis, there is a strong interaction between the incident light and analytes. It is thus expected to greatly enhance the performance of PBGFs based SPR or SER sensors over the conventional ones.

5.6 Chapter Summary

The performance of three types of PBGFs based biochemical sensors has been investigated. It has been found that solid-core PBGFs provide high sensitivity for measuring the high refractive index, which is larger than that of silica. The demonstrated

transmission dips have a wavelength shift of 45nm in response to the refractive index change of 0.01RIU. As the complement, hollow-core PBGFs provide high sensitivity for measuring low refractive index, which is smaller than that of silica. The PBE shifts 110nm when $\Delta n_a=0.02$. In particular, a theoretical analysis has been carried out to investigate the sensitivity for the measurement of the concentration of a specific solution. A surface coverage change $\Gamma_{\min} \approx 3.5 \text{ ng/cm}^2$ has been estimated for the detection of proteins, which is on the same order as other optical methods, such as the SPR method and integrated optical (IO) sensors with grating couplers. These two designs offer the potential for realizing high performance label-free biochemical sensors with simple theoretical models. The applications of the theoretical models can also be extended in the design of evanescent wave sensors. As 95% light interact with samples, the hollow-core PBGFs are ideal for evanescent wave sensing. Without removing the coating, it also offers the convenience of practical applications. Furthermore, the strong interaction of light and sample enables the enhancement of fiber-optic SPR and surface enhanced Raman techniques.

Chapter 6

Conclusions and Future Work

6.1 Summary of the investigation

This thesis reports the results of the investigation on the variations of refractive index induced modifications of photonic bandgaps (PBGs) for both isotropic and anisotropic photonic bandgap fibers (PBGFs). The investigation mainly focuses on finding simple explicit expressions to describe these relationships and afterwards applying these simple formulas in the design of novel PBGFs based biochemical sensors. The work that has been done can be summarized as follows.

In order to understand the relationship between the refractive index and locations of bandgaps for isotropic PBGFs, theoretical models have been developed for both solid-core PBGFs and hollow-core PBGFs, which is validated by numerical results. The guiding mechanism of solid-core PBGFs can be interpreted according to antiresonant optical waveguide (ARROW) model. The locations of the stop bands, which manifest as transmission dips in the transmission spectrum, are related to the cutoff wavelengths of the modes in an individual high-index inclusion. In addition, the widths of these stop bands become gradually broad with the increment of the order of modes. For hollow-core PBGFs, a refractive index scaling law is used to understand the wavelength shifts of the

bandgaps induced by the variation of refractive index. This relationship can be summarized by a simple explicit formula by making the scalar wave approximation. The effect of neglecting the vector part has also been investigated. The scalar wave approximation gives reasonable prediction of the behavior of the PBGs, for the PBGs which are formed without the aid of vectorial effects. The limitation for the scalar wave approximation is that it cannot predict the behavior of the PBGs which are formed by the vectorial effects. However, this does not pose a problem as the device operates at low refractive index contrast, where vectorial effects can be neglectable.

The studies of the anisotropic PBGFs become more complicated, as its refractive index is not homogeneous in all directions. In addition to the scaling of refractive index, the alignment of anisotropic material is the other important issue which can alter the behavior of bandgaps. The investigation of anisotropic PBGFs mainly focuses on the nematic liquid crystal (NLC) infiltrated PBGFs. Similar to the isotropic PBGFs, an ARROW model is proposed for anisotropic solid-core PBGFs and a refractive index scaling law is proposed for anisotropic hollow-core PBGFs. Besides, the effect of NLC alignment has also been investigated, which indicate several novel phenomenon, such as bandgap splitting and hybrid guiding. The unique anisotropic properties also provide several interesting designs of PBGFs. Three configurations of anisotropic PBGFs has been proposed and thoroughly studied, which are grouped according to core and cladding compositions with $n_b < n_o < n_e$, $n_e > n_b > n_o$ and $n_b > n_e > n_o$, respectively. This provides the basic principles for the future biochemical sensors' design.

Experimental studies were carried out to realize the biochemical sensors by using PBGFs and verifying the theoretical models. The solid-core PBGFs are good candidates for the measurement of high refractive index. A 45nm wavelength shift of transmission dip was observed in response to the refractive index change of 0.01RIU. The hollow-core PBGFs can be viewed as a complement to the solid-core PBGFs, which provide the measurement of refractive index ranging from 1.0 to 1.45 assuming the background material is silica. The sensitivity is 110nm wavelength shift with respect to the variation of refractive index of 0.02. In order to evaluate the performance for the measurement of the concentration of a specific solution, a three layers model is proposed. Following the theoretical and numerical results, a surface coverage change $\Gamma_{\min} \approx 3.5 \text{ ng/cm}^2$ has been estimated for the detection of proteins. This result is comparable to the SPR method and IO sensors with grating couplers. Although the theoretical models are mainly focused on the refractive index effect on the bandgap formation, they can be further applied in the design of evanescent wave sensors. According to the refractive index scaling law, it is estimated that more than 95% optical power residing in the holey region, i.e. sample solution. This greatly enhances the effectiveness of the sensing components. In addition, the strong interaction of light and sample enables the enhancement of fiber-optic SPR and surface enhanced Raman techniques.

6.2 Experimental Challenges

Currently, there are two difficult problems for the real applications of the PBGFs based

biochemical sensors. Firstly, it is difficult to couple the light into and out of the PBGFs with low loss. In the PBGF based biochemical sensors, a small section of the PBGF acts as the sensing element. In order to achieve a real-time measurement, the two ends of the PBGF must be left open so that the liquid can flow into and out from the PBGF. Therefore, butt-coupling is the only method to couple the light into and out from the PBGF. However, for this coupling method, only accurate control of the alignment by using high precision translation stages can achieve low loss condition. In order to achieve accurate alignment without using the bulk translation stages, a small section of PCF was incorporated into an optic-fluidic coupler chip to allow the continuous control of liquid flow through the PCF as well as simultaneous optical coupling [65]. The success of the biochip may provide a solution for the optical coupling problem. Secondly, an inevitable loss comes from the scattering impurities of the PBGF, such as air bubbles. In order to reduce this part of loss, a small section of PBGF is preferred to be designed as a sensing element [65, 156, 158].

6.3 Suggestion of Future Work

PBGFs are new fibers and their properties are still being explored. In order to use them as biochemical sensing devices, many issues need to be addressed. Several important issues, especially the fundamental theoretical models, have been studied in this research project. However, due to the time and the technologic limitations, some promising directions were identified but could not be pursued. I have listed the following suggestions for the

future work.

6.3.1 Theoretical Work

6.3.1.1 Symmetry breaking due to alignment of NLC

By now, the idea of constructing a band structure is very familiar by tracing the high symmetry points of the Brillouin zone. However, not all the high symmetry points have been examined. The problem arises with anisotropic materials, even if the shapes in the unit cell have high symmetry [137]. In the present case, the directions of the ordinary and extraordinary axes are not equivalent, and we need to sample a greater portion of the FCC Brillouin zone [137]. A possible approach is to calculate three partial band structures, in which the standard FCC path is used, but the direction of the extraordinary axis is assigned to a different coordinate axis.

6.3.1.2 Nonuniformity

Another issue that has not been investigated is the nonuniformity of NLC. In earlier numerical work, the NLC is assumed to be uniform inside air holes, which leads to a dielectric tensor of NLC independent of location. However, in a generalized approach, the optic axis distribution of a nematic material confined in closed capillary cavities is determined by interplay among the physics of elastic theory, the anchoring conditions at the cavity's surface, and the impact of any external fields [48-49]. Therefore, the alignment of NLC varies with the position, leading to a nonuniformity dielectric tensor of

NLC inside the air holes which is a function of the location.

6.3.1.3 Structure and boundary condition

The boundary condition is determined by the anchoring conditions. The typical kinds of anchoring are (i) monostable homeotropic or normal orientation, (ii) monostable planar or specific tangential orientation, (iii) planar degenerate or orientation anywhere on the plane of the substrate, (iv) oblique degenerate, and (v) conical or orientation anywhere on the plane of the substrate with an oblique angle [50]. Anchoring conditions can be controlled by well-defined chemical and mechanical treatments. For the LC biosensor monostable planar orientation can be created by well-tailored film layers on the glass substrates [50]. On the other hand, protein adsorption on the substrate can change the anchoring condition from monostable to planar degenerate or to conical [50]. In real biosensor devices the anchoring type will be determined by position and a set of length scales [50]. Hence in the biosensor, it is necessary to investigate the degree and spatial distribution of anchoring which indicate the amount of surface adsorbed protein.

6.3.2 Experimental Work

6.3.2.1 Specific Detection

Due to the limitations of time and equipments, the focus of this thesis is to develop theoretical model for the design of PBGFs based biochemical sensors. Several experiments on the non-specific measurements, such as refractive index and fluorescence

experiments on the non-specific measurements, such as refractive index and fluorescence absorption, have been demonstrated for the verification of the theory. In addition, the theoretical background is provided for possible design of a hollow-core PBGFs based biosensor reactive to a specific biochemical agent. The future experimental work is to realize the design experimentally by depositing a bio-layer on the inner surface of the hollow-core PBGFs. In addition, experimental investigation of the LC in response to the presence of the biomolecules will also be conducted in the future work.

6.3.2.2 Fiber on Biochip

One of the major tasks in the future improvements of the design concerns the coupling of the PBGFs and SMFs. A solid optical fiber detects reagents on the outside surface, whereas the reagents are positioned inside the air holes in PBGFs-based biochemical sensors. This poses a problem for the PBGF sensor element, since both fluids and probing electromagnetic waves must enter and exit at the end facets of the fiber. If PBGFs are to be used as more general sensor components, a robust packaging that allows easy coupling to the surrounding optical and fluidic infrastructure is needed.

Author's Publications

Journal papers:

Chapter 4:

1. **J. Sun**, C.C. Chan, P. Shum and C.L. Poh, "Experimental analysis of spectral characteristics of antiresonant guiding photonic crystal fibers", *Optics Letters*, **33**, 809-811, 2008.
2. **J. Sun**, C.C. Chan and X.Y. Dong, "Refractive index measurement by using a photonic crystal fiber", *Optical Engineering*, **46**, 014402/1-014402/4, 2007
3. **J. Sun**, C.C. Chan, X.Y. Dong and P. Shum, "Tunable photonic bandgaps in a photonic crystal fiber filled with low index material", *Journal of Optoelectronics and advanced materials*, **8**, 1593-1596, 2006

Chapter 5:

4. **J. Sun** and C.C. Chan, "Refractive index scaling in liquid-crystal photonic crystal fiber", *Applied Physics B*, under review
5. **J. Sun** and C.C. Chan, "Effect of liquid crystal alignment on bandgap formation in photonic bandgap fibers", *Optics Letters*, **32**, 1989-1991, 2007
6. **J. Sun** and C.C. Chan, "Hybrid guiding in liquid-crystal photonic crystal fibers", *Journal of the Optical Society of America: B, Optical Physics*, **24**, 2640-2646, 2007
7. **J. Sun**, C.C. Chan and N. Ni, "Analysis of photonic crystal fibers infiltrated with nematic liquid crystal", *Optics Communications*, **278**, 66-70, 2007

Chapter 6:

8. **J. Sun**, C.C. Chan, Y.F. Zhang and P. Shum, "Analysis of hollow-core photonic bandgap fibers for evanescent-wave biosensing", *Journal of Biomedical Optics*, **13**, 054048/1-054048/6, 2008. ---selected for the October 15, 2008 issue of *Virtual Journal of Biological Physics Research*

9. **J. Sun**, C.C. Chan and P. Shum, "Antiresonant guiding photonic crystal fibers for measuring refractive index", *Sensors and Actuators: B, Chemical*, under revision
10. **J. Sun**, C.C. Chan, X. Y. Dong, and P. Shum "High resolution photonic bandgap fiber based biochemical sensor", *Journal of Biomedical Optics*, **12**, 044022/1—044022/6, 2007. ---selected for *Virtual Journal of Nanoscale Science & Technology*, vol.16, no.3, 2007 and the July 15, 2007 issue of *Virtual Journal of Biological Physics Research*
11. **J. Sun**, C.C. Chan, X.Y. Dong, and P. Shum, "Photonic bandgap fiber for refractive index measurement", *Sensors and Actuators: B, Chemical*, **128**, 46-50, 2007

Conference papers:

Chapter 4:

1. **J. Sun**, C.C. Chan, X.Y. Dong, and P. Shum, "Tunable photonic bandgaps in a photonic crystal fiber", *SPIE Photonics East 2006*, Boston, USA, 2006
2. **J. Sun**, C.C. Chan, and X.Y. Dong, "Refractive index measurement by using a photonic crystal fiber", *SPIE Photonics West 2006*, San Jose, USA, 2006

Chapter 5:

3. **J. Sun**, C.C. Chan and N. Ni, "Hybrid guiding in liquid-crystal photonic crystal fibers", *Asia-Pacific Optical Communications*, Wuhan, China, 2007
4. **J. Sun**, C.C. Chan, X.Y. Dong and P. Shum, "Photonic bandgap fiber with liquid crystal core for single-polarization single-mode guidance", *4th International Conference on Materials for Advanced Technologies*, Singapore, 2007
5. **J. Sun**, C.C. Chan and N. Ni, "Bandgap formation in nonsilica-glass photonic bandgap fibers with liquid crystal inclusions", *the 7th Pacific Rim Conference on Lasers and Electro-optics (CLEO/Pacific Rim 2007)*, Seoul, Korea, 2007
6. **J. Sun**, C. C. Chan, Y. F. Zhang, "Single polarization guidance in liquid-crystal photonic bandgap fibers", *International Conference on Advanced Infocomm Technology*, Shenzhen, China, 2008

Chapter 6:

7. **J. Sun**, C.C. Chan, Y.F. Zhang and P. Shum, "Analysis of hollow-core photonic bandgap fibers for evanescent-wave biosensing", 6th international conference on Optics-photonics Design & Fabrication, Taipei, Taiwan, 2008
8. **J. Sun**, C.C. Chan, Y.F. Zhang and P. Shum, "Antiresonant guiding photonic crystal fibers for measuring refractive index", 19th international conference on Optical Fiber Sensors (OFS), Perth, Australia, 2008
9. **J. Sun**, C.C. Chan, X.Y. Dong and P. Shum, "High Resolution Biochemical Sensor by Using Photonic Bandgap Fiber," in International Optical Design, Technical Digest (CD) (Optical Society of America, 2006), Vancouver, Canada, 2006

Bibliography

1. "Photonic Crystal Fiber," (Wikipedia, 2008), http://en.wikipedia.org/wiki/Photonic_crystal_fiber
2. P. Prasad, N. "Optical Biosensors," in *Introduction to Biophotonics* (John Wiley & Sons, Inc., Buffalo, NY, USA, 2004), pp. 311-356.
3. F.S. Ligler, and C.A. Rowe-Taitt, *Optical Biosensors: Present and Future* (Elsevier, Amsterdam, 2002).
4. A. Leung, P.M. Shankar, and R. Mutharasan, "A Review of Fiber-Optic Biosensors," *Sens. Actuator B-Chem.* **125**, 688-703 (2007).
5. M. Mehrvar, C. Bis, J.M. Scharer, M. Moo-Young, and J.H. Luong, "Fiber-Optic Biosensors - Trends and Advances," *Anal. Sci.* **16**, 677-692 (2000).
6. A.K. Sharma, R. Jha, and B.D. Gupta, "Fiber-Optic Sensors Based on Surface Plasmon Resonance: A Comprehensive Review," *IEEE Sens. J.* **7**, 1118-1129 (2007).
7. J.M. Fini, "Microstructure Fibres for Optical Sensing in Gases and Liquids," *Meas. Sci. Technol.* **15**, 1120-1128 (2004).
8. L. Kornaszewski, N. Gayraud, J.M. Stone, W.N. MacPherson, A.K. George, J.C. Knight, D.P. Hand, and D.T. Reid, "Mid-Infrared Methane Detection in a Photonic Bandgap Fiber Using a Broadband Optical Parametric Oscillator," *Opt. Express* **15**, 11219-11224 (2007).
9. T. Ritari, J. Tuominen, H. Ludvigsen, J.C. Petersen, T. Sorensen, T.P. Hansen, and H.R. Simonsen, "Gas Sensing Using Air-Guiding Photonic Bandgap Fibers," *Opt. Express* **12**, 4080-4087 (2004).
10. J. Homola, S.S. Yee, and G. Gauglitz, "Surface Plasmon Resonance Sensors: Review," *Sens. Actuator B-Chem.* **54**, 3-15 (1999).
11. P. Lucas, M.R. Riley, C. Boussard-Pledel, and B. Bureau, "Advances in Chalcogenide Fiber Evanescent Wave Biochemical Sensing," *Anal. Biochem.* **351**, 1-10 (2006).

12. J.C. Knight, T.A. Birks, P.S. Russell, and D.M. Atkin, "All-Silica Single-Mode Optical Fiber with Photonic Crystal Cladding," *Opt. Lett.* **21**, 1547-1549 (1996).
13. P. Russell, "Photonic Crystal Fibers," *Science* **299**, 358-362 (2003).
14. P.S.J. Russell, "Photonic-Crystal Fibers," *J. Lightwave Technol.* **24**, 4729-4749 (2006).
15. E. Tapuhi, E.A. Venter, and R. Kfir, "Trends in Biosensor Development and Some Potential Applications," *South African Journal of Chemistry-Suid-Afrikaanse Tydskrif Vir Chemie* **49**, 8-25 (1996).
16. G. Ramsay, *Commercial Biosensors, Applications to Clinical, Bioprocess and Environmental Samples* (John Wiley & Sons, New York, 1998).
17. R.A. Potyrailo, S.E. Hobbs, and G.M. Hieftje, "Optical Waveguide Sensors in Analytical Chemistry: Today's Instrumentation, Applications and Trends for Future Development," *Fresenius Journal of Analytical Chemistry* **362**, 349-373 (1998).
18. J.J. Shi, Y.F. Zhu, X.R. Zhang, W.R.G. Baeyens, and A.M. Garcia-Campana, "Recent Developments in Nanomaterial Optical Sensors," *Trac-Trend Anal. Chem.* **23**, 351-360 (2004).
19. P.C.A. Jeronimo, A.N. Araujo, and M. Montenegro, "Optical Sensors and Biosensors Based on Sol-Gel Films," *Talanta* **72**, 13-27 (2007).
20. J.C. Knight, J. Broeng, T.A. Birks, and P.S.J. Russel, "Photonic Band Gap Guidance in Optical Fibers," *Science* **282**, 1476-1478 (1998).
21. B.J. Eggleton, C. Kerbage, P.S. Westbrook, R.S. Windeler, and A. Hale, "Microstructured Optical Fiber Devices," *Opt. Express* **9**, 698-713 (2001).
22. P. Yeh, A. Yariv, and E. Marom, "Theory of Bragg Fiber," *J. Opt. Soc. Am. B* **68**, 1196-1201 (1978).
23. B. Temelkuran, S.D. Hart, G. Benoit, J.D. Joannopoulos, and Y. Fink, "Wavelength-Scalable Hollow Optical Fibres with Large Photonic Bandgaps for Co₂ Laser Transmission," *Nature* **420**, 650-653 (2002).
24. T.M. Monro, Y.D. West, D.W. Hewak, N.G.R. Broderick, and D.J. Richardson, "Chalcogenide Holey Fibres," *Electron. Lett.* **36**, 1998-2000 (2000).

25. V.V.R.K. Kumar, A. George, J. Knight, and P. Russell, "Tellurite Photonic Crystal Fiber," *Opt. Express* **11**, 2641-2645 (2003).
26. K.M. Kiang, K. Frampton, T.M. Monro, R. Moore, J. Tucknott, D.W. Hewak, D.J. Richardson, and H.N. Rutt, "Extruded Singlemode Non-Silica Glass Holey Optical Fibres," *Electron. Lett.* **38**, 546-547 (2002).
27. M.A. van Eijkelenborg, M.C.J. Large, A. Argyros, J. Zagari, S. Manos, N.A. Issa, I. Bassett, S. Fleming, R.C. McPhedran, C.M. de Sterke, and N.A.P. Nicorovici, "Microstructured Polymer Optical Fibre," *Opt. Express* **9**, 319-327 (2001).
28. S.P.J. Higson, and P.M. Vадgama, "Biosensors - a Viable Monitoring Technology," *Med. Bio. Eng. Comp.* **32**, 601-609 (1994).
29. I. Tinoco, K. Sauer, J.C. Wang, and J.D. Puglisi, *Physical Chemistry: Principles and Applications in Biological Sciences* (Prentice Hall, Englewood Cliffs, NJ, 2001).
30. R.M. Sutherland, C. Dahne, J.F. Place, and A.S. Ringrose, "Optical-Detection of Antibody Antigen Reactions at a Glass Liquid Interface," *Clinic. Chem.* **30**, 1533-1538 (1984).
31. T. Vodinh, B.J. Tromberg, G.D. Griffin, K.R. Ambrose, M.J. Sepaniak, and E.M. Gardenhire, "Antibody-Based Fiberoptics Biosensor for the Carcinogen Benzo(a)Pyrene," *Appl. Spec.* **41**, 735-738 (1987).
32. C. Di Primo, and I. Lebars, "Determination of Refractive Index Increment Ratios for Protein-Nucleic Acid Complexes by Surface Plasmon Resonance," *Anal. Biochem.* **368**, 148-155 (2007).
33. H. Tazawa, T. Kanie, and M. Katayama, "Fiber-Optic Coupler Based Refractive Index Sensor and Its Application to Biosensing," *Appl. Phys. Lett.* **91**, 3 (2007).
34. A. Brecht, J. Ingenhoff, and G. Gauglitz, "Direct Monitoring of Antigen-Antibody Interactions by Spectral Interferometry," *Sens. Actuator B-Chem.* **6**, 96-100 (1992).
35. Y. Liu, P. Hering, and M.O. Scully, "An Integrated Optical Sensor for Measuring Glucose-Concentration," *Appl. Phys. B -Lasers and Opt.* **54**, 18-23 (1992).
36. L.M. Lechuga, A.T.M. Lenferink, R.P.H. Kooyman, and J. Greve, "Feasibility of Evanescent-Wave Interferometer Immunosensors for Pesticide Detection - Chemical Aspects," *Sens. Actuator B-Chem.* **25**, 762-765 (1995).

37. R.G. Heideman, and P.V. Lambeck, "Remote Opto-Chemical Sensing with Extreme Sensitivity: Design, Fabrication and Performance of a Pigtailed Integrated Optical Phase-Modulated Mach-Zehnder Interferometer System," *Sens. Actuator B-Chem.* **61**, 100-127 (1999).
38. B. Liedberg, C. Nylander, and I. Lundstrom, "Biosensing with Surface-Plasmon Resonance - How It All Started," *Biosens. Bioelectron.* **10**, R1-R9 (1995).
39. P. Schuck, "Use of Surface Plasmon Resonance to Probe the Equilibrium and Dynamic Aspects of Interactions between Biological Macromolecules," *Annu. Rev. Biophys. Biomolec. Struct.* **26**, 541-566 (1997).
40. B.D. Spangler, E.A. Wilkinson, J.T. Murphy, and B.J. Tyler, "Comparison of the Spreeta (R) Surface Plasmon Resonance Sensor and a Quartz Crystal Microbalance for Detection of Escherichia Coli Heat-Labile Enterotoxin," *Anal. Chim. Acta* **444**, 149-161 (2001).
41. W.H. Tsai, Y.C. Tsao, H.Y. Lin, and B.C. Shen, "Cross-Point Analysis for a Multimode Fiber Sensor Based on Surface Plasmon Resonance," *Opt. Lett.* **30**, 2209-2211 (2005).
42. J.H. Holtz, and S.A. Asher, "Polymerized Colloidal Crystal Hydrogel Films as Intelligent Chemical Sensing Materials," *Nature* **389**, 829-832 (1997).
43. J.H. Holtz, J.S.W. Holtz, C.H. Munro, and S.A. Asher, "Intelligent Polymerized Crystalline Colloidal Arrays: Novel Chemical Sensor Materials," *Anal. Chem.* **70**, 780-791 (1998).
44. C.E. Reese, M.E. Baltusavich, J.P. Keim, and S.A. Asher, "Development of an Intelligent Polymerized Crystalline Colloidal Array Colorimetric Reagent," *Anal. Chem.* **73**, 5038-5042 (2001).
45. V. Alexeev, A. Sharma, I. Lednev, C. Wilcox, D. Finegold, and S.A. Asher, "Intelligent Polymerized Crystalline Colloidal Array Photonic Crystal Glucose Sensors," *Abstr. Pap. Am. Chem. Soc.* **224**, U116-U116 (2002).
46. S.A. Asher, S.F. Peteu, C.E. Reese, M.X. Lin, and D. Finegold, "Polymerized Crystalline Colloidal Array Chemical-Sensing Materials for Detection of Lead in Body Fluids," *Anal. Bioanal. Chem.* **373**, 632-638 (2002).
47. V.K. Gupta, J.J. Skaife, T.B. Dubrovsky, and N.L. Abbott, "Optical Amplification of Ligand-Receptor Binding Using Liquid Crystals," *Science* **279**, 2077-2080 (1998).

-
48. J.J. Skaife, and N.L. Abbott, "Quantitative Interpretation of the Optical Textures of Liquid Crystals Caused by Specific Binding of Immunoglobulins to Surface-Bound Antigens," *Langmuir* **16**, 3529-3536 (2000).
49. J.J. Skaife, and N.L. Abbott, "Influence of Molecular-Level Interactions on the Orientations of Liquid Crystals Supported on Nanostructured Surfaces Presenting Specifically Bound Proteins," *Langmuir* **17**, 5595-5604 (2001).
50. D.K. Hwang, and A.D. Rey, "Optical Modeling of Liquid Crystal Biosensors," *J. Chem. Phys.* **125**, 9 (2006).
51. B.P. Nelson, T.E. Grimsrud, M.R. Liles, R.M. Goodman, and R.M. Corn, "Surface Plasmon Resonance Imaging Measurements of DNA and Rna Hybridization Adsorption onto DNA Microarrays," *Anal. Chem.* **73**, 1-7 (2001).
52. W. Lukosz, "Principles and Sensitivities of Integrated Optical and Surface-Plasmon Sensors for Direct Affinity Sensing and Immunosensing," *Biosens. Bioelectron.* **6**, 215-225 (1991).
53. M.P. DeLisa, Z. Zhang, M. Shiloach, S. Pilevar, C.C. Davis, J.S. Sirkis, and W.E. Bentley, "Evanescent Wave Long Period Fiber Bragg Grating as an Immobilized Antibody Biosensor," *Anal. Chem.* **72**, 2895-2900 (2000).
54. Z. Zhang, "Development of Optical Fiber Biosensors with Long Period Gratings," (University of Maryland, Colledge Park, 2000).
55. E. Chow, A. Grot, L.W. Mirkarimi, M. Sigalas, and G. Girolami, "Ultracompact Biochemical Sensor Built with Two-Dimensional Photonic Crystal Microcavity," *Opt. Lett.* **29**, 1093-1095 (2004).
56. V.N. Konopsky, and E.V. Alieva, "Photonic Crystal Surface Waves for Optical Biosensors," *Anal. Chem.* **79**, 4729-4735 (2007).
57. M. Lee, and P.M. Fauchet, "Two-Dimensional Silicon Photonic Crystal Based Biosensing Platform for Protein Detection," *Opt. Express* **15**, 4530-4535 (2007).
58. J.P. Walker, K.W. Kimble, and S.A. Asher, "Photonic Crystal Sensor for Organophosphate Nerve Agents Utilizing the Organophosphorus Hydrolase Enzyme," *Anal. Bioanal. Chem.* **389**, 2115-2124 (2007).
59. R.P. Haugland, *The Handbook—a Guide to Fluorescent Probes and Labeling Technologies* (Molecular Probes, Eugene, OR, 2005).

60. V. Bhatia, and A.M. Vengsarkar, "Optical Fiber Long-Period Grating Sensors," *Opt. Lett.* **21**, 692-694 (1996).
61. H.J. Patrick, A.D. Kersey, and F. Bucholtz, "Analysis of the Response of Long Period Fiber Gratings to External Index of Refraction," *J. Lightwave Technol.* **16**, 1606-1612 (1998).
62. S.W. James, and R.P. Tatam, "Optical Fibre Long-Period Grating Sensors: Characteristics and Application," *Meas. Sci. Technol.* **14**, R49-R61 (2003).
63. K.L. Brogan, and D.R. Walt, "Optical Fiber-Based Sensors: Application to Chemical Biology," *Current Opinion in Chemical Biology* **9**, 494-500 (2005).
64. O.S. Wolfbeis, "Fiber-Optic Chemical Sensors and Biosensors," *Anal. Chem.* **78**, 3859-3873 (2006).
65. L. Rindorf, P.E. Hoiby, J.B. Jensen, L.H. Pedersen, O. Bang, and O. Geschke, "Towards Biochips Using Microstructured Optical Fiber Sensors," *Anal. Bioanal. Chem.* **385**, 1370-1375 (2006).
66. K. Lee, and S.A. Asher, "Photonic Crystal Chemical Sensors: Ph and Ionic Strength," *Journal of the American Chemical Society* **122**, 9534-9537 (2000).
67. S.J. Woltman, G.D. Jay, and G.P. Crawford, "Liquid-Crystal Materials Find a New Order in Biomedical Applications," *Nature Materials* **6**, 929-938 (2007).
68. G. Keiser, *Optical Fiber Communications* (McGraw-Hill, Columbus, OH 2000).
69. A.B. John, *Fundamentals of Optical Fibers* (Wiley-Interscience, New York, NY, 2004).
70. A.W. Snyder, and J.D. Love, *Optical Waveguide Theory* (Chapman & Hall, London, 1983).
71. S. Shalem, A. Tsun, E. Rave, A. Millo, L. Nagli, and A. Katzir, "Silver Halide Single-Mode Fibers for the Middle Infrared," *Appl. Phys. Lett.* **87**, 3 (2005).
72. P. Lucas, M.A. Solis, D. Le Coq, C. Juncker, M.R. Riley, J. Collier, D.E. Boesewetter, C. Boussard-Pledel, and B. Bureau, "Infrared Biosensors Using Hydrophobic Chalcogenide Fibers Sensitized with Live Cells," *Sens. Actuator B-Chem.* **119**, 355-362 (2006).

-
73. R. Gotz, B. Mizaikoff, and R. Kellner, "Application of Sapphire Fibers to an Ir Fiber-Optic Sensor for the Investigation of Polymers at Elevated Temperature," *Appl. Spec.* **52**, 1248-1252 (1998).
74. J.C. Knight, and D.V. Skryabin, "Nonlinear Waveguide Optics and Photonic Crystal Fibers," *Opt. Express* **15**, 15365-15376 (2007).
75. D.H. Kim, and J.U. Kang, "Analysis of Temperature-Dependent Birefringence of a Polarization-Maintaining Photonic Crystal Fiber," *Opt. Eng.* **46**, 5 (2007).
76. Y. Yue, G.Y. Kai, Z. Wang, T.T. Sun, L. Jin, Y.F. Lu, C.S. Zhang, L.G. Liu, Y. Li, Y.G. Liu, S.Z. Yuan, and X.Y. Dong, "Highly Birefringent Elliptical-Hole Photonic Crystal Fiber with Squeezed Hexagonal Lattice," *Opt. Lett.* **32**, 469-471 (2007).
77. H.B. Li, A. Mafi, A. Schulzgen, L. Li, V.L. Temyanko, N. Peyghambarian, and J.V. Moloney, "Analysis and Design of Photonic Crystal Fibers Based on an Improved Effective-Index Method," *J. Lightwave Technol.* **25**, 1224-1230 (2007).
78. V.P. Mitrokhin, A.A. Ivanov, A.B. Fedotov, M.V. Alfimov, K.V. Dukel'skii, A.V. Khokhlov, V.S. Shevandin, Y.N. Kondrat'ev, A.A. Podshivalov, and A.M. Zheltikov, "Spectral Transformation of Megawatt Femtosecond Optical Pulses in Large-Mode-Area High-Index-Step Photonic-Crystal Fibers," *Laser Phys. Lett.* **4**, 529-533 (2007).
79. R.F. Cregan, B.J. Mangan, J.C. Knight, T.A. Birks, P.S. Russell, P.J. Roberts, and D.C. Allan, "Single-Mode Photonic Band Gap Guidance of Light in Air," *Science* **285**, 1537-1539 (1999).
80. C.J. Hensley, D.H. Broaddus, C.B. Schaffer, and A.L. Gaeta, "Photonic Band-Gap Fiber Gas Cell Fabricated Using Femtosecond Micromachining," *Opt. Express* **15**, 6690-6695 (2007).
81. S.G. Li, S.Y. Liu, Z.Y. Song, Y. Han, T.L. Cheng, G.Y. Zhou, and L.T. Hou, "Study of the Sensitivity of Gas Sensing by Use of Index-Guiding Photonic Crystal Fibers," *Appl. Optics* **46**, 5183-5188 (2007).
82. J.D. Joannopoulos, R.D. Meade, and J.N. Winn, *Photonic Crystals: Molding the Flow of Light* (Princeton University Press, Princeton, NJ, 1995).
83. F.M. Cox, R. Lwin, M.C.J. Large, and C.M.B. Cordeiro, "Opening up Optical Fibres," *Opt. Express* **15**, 11843-11848 (2007).

-
84. B. Bahadur, *Liquid Crystals: Applications and Uses* (World Scientific, Singapore, 1990).
85. K. Kawano, and T. Kitoh, *Introduction to Optical Waveguide Analysis: Solving Maxwell's Equation and the Schrödinger Equation* (Wiley-Interscience, New York, 2001).
86. D.K. Cheng, *Field and Wave Electromagnetics* (Addison-Wesley Publishing Company, Inc, 1989).
87. M. Yan, "Lightwave Propagation in Microstructured Optical Fibers," in *School of Electrical and Electronic Engineering*(Nanyang Technological University, Singapore, 2005).
88. K.M. Ho, C.T. Chan, and C.M. Soukoulis, "Existence of a Photonic Gap in Periodic Dielectric Structures," *Phys. Rev. Lett.* **65**, 3152-3155 (1990).
89. K.M. Leung, and Y.F. Liu, "Photon Band Structures - the Plane-Wave Method," *Phys. Rev. B* **41**, 10188-10190 (1990).
90. S.G. Johnson, and J.D. Joannopoulos, "Block-Iterative Frequency-Domain Methods for Maxwell's Equations in a Planewave Basis," *Opt. Express* **8**, 173-190 (2001).
91. Z.M. Zhu, and T.G. Brown, "Analysis of the Space Filling Modes of Photonic Crystal Fibers," *Opt. Express* **8**, 547-554 (2001).
92. B.J. Eggleton, A.K. Ahuja, K.S. Feder, C. Headley, C. Kerbage, M.D. Mermelstein, J.A. Rogers, P. Steinvurzel, P.S. Westbrook, and R.S. Windeler, "Novel Waveguide Structures for Enhanced Fiber Grating Devices," *IEEE J. Sel. Top. Quantum Electron.* **7**, 409-424 (2001).
93. B.J. Eggleton, P.S. Westbrook, R.S. Windeler, S. Spalter, and T.A. Strasser, "Grating Resonances in Air-Silica Microstructured Optical Fibers," *Opt. Lett.* **24**, 1460-1462 (1999).
94. W.P. Huang, and C.L. Xu, "Simulation of 3-Dimensional Optical Wave-Guides by a Full-Vector Beam-Propagation Method," *IEEE J. Quantum Electron.* **29**, 2639-2649 (1993).
95. C.L. Xu, W.P. Huang, J. Chrostowski, and S.K. Chaudhuri, "A Full-Vectorial Beam-Propagation Method for Anisotropic Wave-Guides," *J. Lightwave Technol.* **12**, 1926-1931 (1994).

96. P. Lusse, P. Stuwe, J. Schule, and H.G. Unger, "Analysis of Vectorial Mode Fields in Optical Wave-Guides by a New Finite-Difference Method," *J. Lightwave Technol.* **12**, 487-494 (1994).
97. G.R. Hadley, and R.E. Smith, "Full-Vector Wave-Guide Modeling Using an Iterative Finite-Difference Method with Transparent Boundary-Conditions," *J. Lightwave Technol.* **13**, 465-469 (1995).
98. Y.C. Chiang, Y.P. Chiou, and H.C. Chang, "Improved Full-Vectorial Finite-Difference Mode Solver for Optical Waveguides with Step-Index Profiles," *J. Lightwave Technol.* **20**, 1609-1618 (2002).
99. Z.M. Zhu, and T.G. Brown, "Full-Vectorial Finite-Difference Analysis of Microstructured Optical Fibers," *Opt. Express* **10**, 853-864 (2002).
100. F. Brechet, J. Marcou, D. Pagnoux, and P. Roy, "Complete Analysis of the Characteristics of Propagation into Photonic Crystal Fibers, by the Finite Element Method," *Optical Fiber Tech.* **6**, 181-191 (2000).
101. K. Saitoh, and M. Koshiba, "Full-Vectorial Imaginary-Distance Beam Propagation Method Based on a Finite Element Scheme: Application to Photonic Crystal Fibers," *IEEE J. Quantum Electron.* **38**, 927-933 (2002).
102. H.P. Uranus, and H. Hoekstra, "Modelling of Microstructured Waveguides Using a Finite-Element-Based Vectorial Mode Solver with Transparent Boundary Conditions," *Opt. Express* **12**, 2795-2809 (2004).
103. B.T. Kuhlmeiy, T.P. White, G. Renversez, D. Maystre, L.C. Botten, C.M. de Sterke, and R.C. McPhedran, "Multipole Method for Microstructured Optical Fibers. Ii. Implementation and Results," *J. Opt. Soc. Am. B* **19**, 2331-2340 (2002).
104. T.P. White, B.T. Kuhlmeiy, R.C. McPhedran, D. Maystre, G. Renversez, C.M. de Sterke, and L.C. Botten, "Multipole Method for Microstructured Optical Fibers. I. Formulation," *J. Opt. Soc. Am. B* **19**, 2322-2330 (2002).
105. D. Mogilevtsev, T.A. Birks, and P.S. Russell, "Localized Function Method for Modeling Defect Modes in 2-D Photonic Crystals," *J. Lightwave Technol.* **17**, 2078-2081 (1999).
106. T.M. Monro, D.J. Richardson, N.G.R. Broderick, and P.J. Bennett, "Holey Optical Fibers: An Efficient Modal Model," *J. Lightwave Technol.* **17**, 1093-1102 (1999).

-
107. E. Silvestre, M.V. Andres, and P. Andres, "Biorthonormal-Basis Method for the Vector Description of Optical-Fiber Modes," *J. Lightwave Technol.* **16**, 923-928 (1998).
108. A. Ferrando, E. Silvestre, J.J. Miret, P. Andres, and M.V. Andres, "Full-Vector Analysis of a Realistic Photonic Crystal Fiber," *Opt. Lett.* **24**, 276-278 (1999).
109. T.A. Birks, J.C. Knight, and P.S. Russell, "Endlessly Single-Mode Photonic Crystal Fiber," *Opt. Lett.* **22**, 961-963 (1997).
110. A. Bjarklev, and J. Broeng, *Photonic Crystal Fibres* (Springer, 2003).
111. F. Zolla, G. Renversez, A. Nicolet, B.T. Kuhlmeiy, S. Guenneau, and D. Felbacq, *Foudations of Photonic Crystal Fibres* (Imperial College Press, London, 2005).
112. G. Alagappan, X.W. Sun, P. Shum, M.B. Yu, and D. den Engelsen, "Symmetry Properties of Two-Dimensional Anisotropic Photonic Crystals," *J. Opt. Soc. Am. A* **23**, 2002-2013 (2006).
113. S. Guo, "Photonic Crystals: Modeling and Simulation," (Old Dominion University, 2004).
114. Y. Tsuji, M. Koshiba, and N. Takimoto, "Finite Element Beam Propagation Method for Anisotropic Optical Waveguides," *J. Lightwave Technol.* **17**, 723-728 (1999).
115. K. Saitoh, and M. Koshiba, "Approximate Scalar Finite-Element Beam-Propagation Method with Perfectly Matched Layers for Anisotropic Optical Waveguides," *J. Lightwave Technol.* **19**, 786-792 (2001).
116. N.M. Litchinitser, A.K. Abeeluck, C. Headley, and B.J. Eggleton, "Antiresonant Reflecting Photonic Crystal Optical Waveguides," *Opt. Lett.* **27**, 1592-1594 (2002).
117. N.A. Issa, "Modes and Propagation in Microstructured Optical Fibre," (University of Sydney, Australia, 2005).
118. N.M. Litchinitser, S.C. Dunn, P.E. Steinvurzel, B.J. Eggleton, T.P. White, R.C. McPhedran, and C.M. de Sterke, "Application of an Arrow Model for Designing Tunable Photonic Devices," *Opt. Express* **12**, 1540-1550 (2004).
119. A. Argyros, T.A. Birks, S.G. Leon-Saval, C.M.B. Cordeiro, and P.S. Russell, "Guidance Properties of Low-Contrast Photonic Bandgap Fibres," *Opt. Express* **13**, 2503-2511 (2005).

-
120. G. Renversez, P. Boyer, and A. Sagrini, "Antiresonant Reflecting Optical Waveguide Microstructured Fibers Revisited: A New Analysis Based on Leaky Mode Coupling," *Opt. Express* **14**, 5682-5687 (2006).
121. M.A. Duguay, Y. Kokubun, T.L. Koch, and L. Pfeiffer, "Antiresonant Reflecting Optical Waveguides in SiO_2 -Si Multilayer Structures," *Appl. Phys. Lett.* **49**, 13-15 (1986).
122. J. Laegsgaard, "Gap Formation and Guided Modes in Photonic Bandgap Fibres with High-Index Rods," *J. Opt. A-Pure Appl. Opt.* **6**, 798-804 (2004).
123. T.P. White, R.C. McPhedran, C.M. de Sterke, N.M. Litchinitser, and B.J. Eggleton, "Resonance and Scattering in Microstructured Optical Fibers," *Opt. Lett.* **27**, 1977-1979 (2002).
124. N.M. Litchinitser, S.C. Dunn, B. Usner, B.J. Eggleton, T.P. White, R.C. McPhedran, and C.M. de Sterke, "Resonances in Microstructured Optical Waveguides," *Opt. Express* **11**, 1243-1251 (2003).
125. M. Abramowitz, and I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (Dover, New York, 1964).
126. T.A. Birks, D.M. Bird, T.D. Hedley, J.M. Pottage, and P.S. Russell, "Scaling Laws and Vector Effects in Bandgap-Guiding Fibres," *Opt. Express* **12**, 69-74 (2004).
127. J. Sun, C.C. Chan, X.Y. Dong, and P. Shum, "Tunable Photonic Band Gaps in a Photonic Crystal Fiber Filled with Low Index Material," *Journal of Optoelectronics and Advanced Materials* **8**, 1593-1596 (2006).
128. T.T. Larsen, A. Bjarklev, D.S. Hermann, and J. Broeng, "Optical Devices Based on Liquid Crystal Photonic Bandgap Fibres," *Opt. Express* **11**, 2589-2596 (2003).
129. T.T. Alkeskjold, J. Laegsgaard, A. Bjarklev, D.S. Hermann, Anawati, J. Broeng, J. Li, and S.T. Wu, "All-Optical Modulation in Dye-Doped Nematic Liquid Crystal Photonic Bandgap Fibers," *Opt. Express* **12**, 5857-5871 (2004).
130. J. Sun, and C.C. Chan, "Effect of Liquid Crystal Alignment on Bandgap Formation in Photonic Bandgap Fibers," *Opt. Lett.* **32**, 1989-1991 (2007).
131. J. Sun, C.C. Chan, and N. Ni, "Analysis of Photonic Crystal Fibers Infiltrated with Nematic Liquid Crystal," *Opt. Commun.* **278**, 66-70 (2007).

132. C.R. Rosberg, F.H. Bennet, D.N. Neshev, P.D. Rasmussen, O. Bang, W. Krolikowski, A. Bjarklev, and Y.S. Kivshar, "Tunable Diffraction and Self-Defocusing in Liquid-Filled Photonic Crystal Fibers," *Opt. Express* **15**, 12145-12150 (2007).
133. J. Sun, and C.C. Chan, "Hybrid Guiding in Liquid-Crystal Photonic Crystal Fibers," *J. Opt. Soc. Am. B* **24**, 2640-2646 (2007).
134. T.R. Wolinski, S. Ertman, A. Czapla, P. Lesiak, K. Nowecka, A. Wdomanski, E. Nowinowski-Kruszelnicki, R. Dabrowski, and J. Wojcik, "Polarization Effects in Photonic Liquid Crystal Fibers," *Meas. Sci. Technol.* **18**, 3061-3069 (2007).
135. J. Li, and S.T. Wu, "Extended Cauchy Equations for the Refractive Indices of Liquid Crystals," *J. Appl. Phys.* **95**, 896-901 (2004).
136. M. Koshiba, K. Hayata, and M. Suzuki, "Approximate Scalar Finite-Element Analysis of Anisotropic Optical-Waveguides with Off-Diagonal Elements in a Permittivity Tensor," *IEEE Trans. Microwave Theory Tech.* **32**, 587-593 (1984).
137. S. John, and K. Busch, "Photonic Bandgap Formation and Tunability in Certain Self-Organizing Systems," *J. Lightwave Technol.* **17**, 1931-1943 (1999).
138. M. Feng, A.K. Mairaj, D.W. Hewak, and T.M. Monro, "Nonsilica Glasses for Holey Fibers," *J. Lightwave Technol.* **23**, 2046-2054 (2005).
139. M. Yan, and P. Shum, "Air-Guiding Photonic Bandgap Fiber with Improved Triangular Air-Silica Photonic Crystal Cladding," in *Optical Communication, 2005. ECOC 2005. 31st European Conference on*(2005), pp. 689-690 vol.683.
140. G. Antonopoulos, F. Benabid, T.A. Birks, D.M. Bird, J.C. Knight, and P.S.J. Russell, "Experimental Demonstration of the Frequency Shift of Bandgaps in Photonic Crystal Fibers Due to Refractive Index Scaling," *Opt. Express* **14**, 3000-3006 (2006).
141. J.D. Dai, and C.K. Jen, "Analysis of Cladded Uniaxial Single-Crystal Fibers," *J. Opt. Soc. Am. A* **8**, 2021 (1991).
142. B. Ryan, R.S. Windeler, K.S. Kranz, C. Kerbage, and B.J. Eggleton, "Tunable Photonic Band Gap Fiber," in *Optical Fiber Communications Conference*(Optical Society of America, 2002), p. ThK3.
143. C.S. Zhang, G.Y. Kai, Z. Wang, T.T. Sun, C. Wang, Y.G. Liu, J.F. Liu, W.G. Zhang, S.Z. Yuan, and X.Y. Dong, "Design of Tunable Bandgap Guidance in High-Index Filled Microstructure Fibers," *J. Opt. Soc. Am. B* **23**, 782-786 (2006).

144. D.C. Bownass, J.S. Barton, and J.D.C. Jones, "Serially Multiplexed Point Sensor for the Detection of High Humidity in Passive Optical Networks," *Opt. Lett.* **22**, 346-348 (1997).
145. M. Shadaram, J.J. Martinez, F. Garcia, D. Tavares, A. Symon, N. Godbout, and S. Lacroix, "Application of Ferrocene-Based Polymers as Variable Index Materials in Fiber Optic Gas Sensors," in *Functional Photonic and Fiber Devices*(SPIE, San Jose, CA, USA, 1996), pp. 164-168.
146. J.B. Jensen, L.H. Pedersen, P.E. Hoiby, L.B. Nielsen, T.P. Hansen, J.R. Folkenberg, J. Riishede, D. Noordegraaf, K. Nielsen, A. Carlsen, and A. Bjarklev, "Photonic Crystal Fiber Based Evanescent-Wave Sensor for Detection of Biomolecules in Aqueous Solutions," *Opt. Lett.* **29**, 1974-1976 (2004).
147. W.S. Pegau, D. Gray, and J.R.V. Zaneveld, "Absorption and Attenuation of Visible and near-Infrared Light in Water: Dependence on Temperature and Salinity," *Appl. Optics* **36**, 6035-6046 (1997).
148. F.M. Sogandares, and E.S. Fry, "Absorption Spectrum (340-640nm) of Pure Water. I. Photothermal Measurements," *Appl. Opt.* **36**, 8699-8709 (1997).
149. "Introduction to Optical Liquids," (Cargille Labs), <http://www.cargille.com/opticalintro.shtml>.
150. C. Fattinger, H. Koller, D. Schlatter, and P. Wehrli, "The Difference Interferometer - a Highly Sensitive Optical Probe for Quantification of Molecular-Surface Concentration," *Biosens. Bioelectron.* **8**, 99-107 (1993).
151. J.B. Jensen, P.E. Hoiby, G. Emiliyanov, O. Bang, L.H. Pedersen, and A. Bjarklev, "Selective Detection of Antibodies in Microstructured Polymer Optical Fibers," *Opt. Express* **13**, 5883-5889 (2005).
152. J. Sun, and C.C. Chan, "Photonic Bandgap Fiber for Refractive Index Measurement," *Sens. Actuator B-Chem.* **128**,46-50, (2007).
153. J. Sun, C.C. Chan, X.Y. Dong, and P. Shum, "High-Resolution Photonic Bandgap Fiber-Based Biochemical Sensor," *J. Biomed. Opt.* **12**, 044022-044026 (2007).
154. F.M. Cox, A. Argyros, and M.C.J. Large, "Liquid-Filled Hollow Core Microstructured Polymer Optical Fiber," *Opt. Express* **14**, 4135-4140 (2006).

155. C. Martelli, J. Canning, D. Stocks, and M.J. Crossley, "Water-Soluble Porphyrin Detection in a Pure-Silica Photonic Crystal Fiber," *Opt. Lett.* **31**, 2100-2102 (2006).
156. S. Smolka, M. Barth, and O. Benson, "Highly Efficient Fluorescence Sensing with Hollow Core Photonic Crystal Fibers," *Opt. Express* **15**, 12783-12791 (2007).
157. C. Wohlfarth, and M.D. Lechner, *Refractive Indices of Pure Liquids and Binary Liquid Mixtures* (Springer, New York, 2008).
158. L. Rindorf, J.B. Jensen, M. Dufva, L.H. Pedersen, P.E. Hoiby, and O. Bang, "Photonic Crystal Fiber Long-Period Gratings for Biochemical Sensing," *Opt. Express* **14**, 8224-8231 (2006).
159. M. Lelek, F. Louradour, V. Couderc, P. Viale, S. Fevrier, J.L. Auguste, J.M. Blondy, and A. Barthelemy, "High Sensitivity Autocorrelator Based on a Fluorescent Liquid Core Fiber," *Appl. Phys. Lett.* **89** (2006).
160. B. Gauvreau, A. Hassani, M.F. Fehri, A. Kabashin, and M. Skorobogatiy, "Photonic Bandgap Fiber-Based Surface Plasmon Resonance Sensors," *Opt. Express* **15**, 11413-11426 (2007).
161. M. Hautakorpi, M. Mattinen, and H. Ludvigsen, "Surface-Plasmon-Resonance Sensor Based on Three-Hole Microstructured Optical Fiber," *Opt. Express* **16**, 8427-8432 (2008).
162. F.M. Cox, A. Argyros, M.C.J. Large, and S. Kalluri, "Surface Enhanced Raman Scattering in a Hollow Core Microstructured Optical Fiber," *Opt. Express* **15**, 13675-13681 (2007).
163. H. Yan, J. Liu, C.X. Yang, G.F. Jin, C. Gu, and L. Hou, "Novel Index-Guided Photonic Crystal Fiber Surface-Enhanced Raman Scattering Probe," *Opt. Express* **16**, 8300-8305 (2008).